

## Adhesion Mechanism of Water Droplets on Hierarchically Rough Superhydrophobic Rose Petal Surface

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Energy and Process Engineering, Engineering materials science and solutions (EMASS)

Contributors: Teisala, H., Tuominen, M., Kuusipalo, J.

Number of pages: 6

Pages: 1-6

Publication date: 2011

Peer-reviewed: Yes

### Publication information

Journal: Journal of Nanomaterials

Volume: 2011

Article number: 818707

ISSN (Print): 1687-4110

Ratings:

Scopus rating (2011): CiteScore 1.3 SJR 0.437 SNIP 0.478

Original language: English

DOIs:

10.1155/2011/818707

### Bibliographical note

Contribution: organisation=epr pap,FACT1=1

Source: researchoutputwizard

Source ID: 7362

Research output: Contribution to journal › Article › Scientific › peer-review

## Adhesion of Extrusion-Coated Polymer Sealing Layers to a Fiber-Based Packaging Material with an Atomic Layer Deposited Aluminum Oxide Surface Coating

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Energy and Process Engineering

Contributors: Lahtinen, K., Johansson, P., Kääriäinen, T., Cameron, D. C.

Pages: 1985-1990

Publication date: 2012

Peer-reviewed: Yes

### Publication information

Journal: Polymer Engineering and Science

Volume: 52

Issue number: 9

ISSN (Print): 0032-3888

Ratings:

Scopus rating (2012): CiteScore 2.4 SJR 0.688 SNIP 1.283

Original language: English

DOIs:

10.1002/pen.23148

URLs:

<http://onlinelibrary.wiley.com/doi/10.1002/pen.23148/abstract>

### Bibliographical note

Article first published online: 27 MAR 2012  
Contribution: organisation=epr,FACT1=1  
Publisher name: John Wiley & Sons, Inc.

Source: researchoutputwizard

Source ID: 4624

Research output: Contribution to journal › Article › Scientific › peer-review

## Atmospheric synthesis of superhydrophobic TiO<sub>2</sub> nanoparticle deposits in a single step using Liquid Flame Spray

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research area: Aerosol Physics, Department of Materials Science, Department of Physics, Department of Energy and Process Engineering, Engineering materials science and solutions (EMASS), Urban circular bioeconomy (UrCirBio)

Contributors: Aromaa, M., Arffman, A., Suhonen, H., Haapanen, J., Keskinen, J., Honkanen, M., Nikkanen, J., Levänen, E., Messing, M., Deppert, K., Teisala, H., Tuominen, M., Kuusipalo, J., Stepien, M., Saarinen, J., Toivakka, M., Mäkelä, J. M.

Pages: 57-68

Publication date: 2012

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Aerosol Science

Volume: 52

ISSN (Print): 0021-8502

Ratings:

Scopus rating (2012): CiteScore 4.8 SJR 1.284 SNIP 1.594

Original language: English

DOIs:

10.1016/j.jaerosci.2012.04.009

#### Bibliographical note

Contribution: organisation=fys,FACT1=0.34  
Contribution: organisation=mol,FACT2=0.33  
Contribution: organisation=epr,FACT3=0.33  
Publisher name: Pergamon Press

Source: researchoutputwizard

Source ID: 3864

Research output: Contribution to journal › Article › Scientific › peer-review

### Atomic layer deposition on polymer based flexible packaging materials: Growth characteristics and diffusion barrier properties

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Energy and Process Engineering, Engineering materials science and solutions (EMASS)

Contributors: Kääriäinen, T. O., Maydannik, P., Cameron, D. C., Lahtinen, K., Johansson, P., Kuusipalo, J.

Pages: 3146-3154

Publication date: 2011

Peer-reviewed: Yes

#### Publication information

Journal: Thin Solid Films

Volume: 519

Issue number: 10

ISSN (Print): 0040-6090

Ratings:

Scopus rating (2011): CiteScore 3.4 SJR 0.995 SNIP 1.323

Original language: English

DOIs:

10.1016/j.tsf.2010.12.171

#### Bibliographical note

Contribution: organisation=epr pap,FACT1=1  
Publisher name: Elsevier

Source: researchoutputwizard

Source ID: 6254

Research output: Contribution to journal › Article › Scientific › peer-review

### Bio-Hybrid Nanocomposite Coatings from Sonicated Chitosan and Nanoclay

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Energy and Process Engineering

Contributors: Vartiainen, J., Tuominen, M., Nättinen, K.

Pages: 3638-3647  
Publication date: 2010  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Applied Polymer Science  
Volume: 116  
Issue number: 6  
ISSN (Print): 0021-8995  
Ratings:  
Scopus rating (2010): SJR 0.685 SNIP 0.915  
Original language: English  
DOIs:  
10.1002/app.31922

#### Bibliographical note

Contribution: organisation=epr pap,FACT1=1  
Source: researchoutputwizzard  
Source ID: 9532  
Research output: Contribution to journal > Article > Scientific > peer-review

#### Characterization of endoglucanase rich *Trichoderma reesei* cellulase mixtures and their effect on alkaline solubility of dissolving pulp

Dissolving grade pulps are used to manufacture regenerated cellulosic fibres. One promising process for the production of regenerated fibres utilises endoglucanase rich cellulases in the modification of dissolving pulp into alkaline soluble form. The aim of this paper was to characterise cellulases produced by *Trichoderma reesei* that are available in large quantities and study their effect on the dissolving grade softwood pulp, especially on its alkaline solubility. All the studied cellulases had endoglucanase activity and they decreased the intrinsic viscosity of the pulp. The degradation of cellulose into solubilised sugars increased with the cellulases containing also cellobiohydrolases. The monocomponent endoglucanases enhanced alkaline solubility of the pulp more than the multicomponent cellulases and produced alkaline solutions with higher fluidity. The studies showed that the type of the cellulases in the enzyme mixture has significant effect on the amount of solubilised sugars during the enzyme treatment and on the alkaline solubility of the pulp.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Department of Materials Science, Biomass Processing Technologies, VTT Technical Research Centre of Finland, Lappeenranta University of Technology, Stora Enso  
Contributors: Kamppuri, T., Vehviläinen, M., Backfolk, K., Heiskanen, I.  
Number of pages: 11  
Pages: 3901–3911  
Publication date: Dec 2016  
Peer-reviewed: Yes  
Early online date: 30 Aug 2016

#### Publication information

Journal: Cellulose  
Volume: 23  
Issue number: 6  
ISSN (Print): 0969-0239  
Ratings:  
Scopus rating (2016): CiteScore 6.1 SJR 1.146 SNIP 1.196  
Original language: English  
ASJC Scopus subject areas: Polymers and Plastics  
Keywords: Alkaline solubility, Cellulase, Cellulose, Endoglucanase, *Trichoderma reesei*  
DOIs:  
10.1007/s10570-016-1055-2  
Source: Scopus  
Source ID: 84984846328  
Research output: Contribution to journal > Article > Scientific > peer-review

#### Charge Shift/Recombination and Triplet Formation in a Closely-Spaced Molecular Dyad based on a Borondipyrromethene (Bodipy) and an Expanded Acridinium Cation

A molecular monocationic dyad comprising a borondipyrromethene (Bodipy) and an expanded planar acridinium cation was prepared. The dyad, when excited in solution by an ultrashort laser pulse, generates a charge-shift state, where a

positive charge is transferred to the Bodipy from the acridinium subunit. The process takes less than 1 ps in MeCN and around 8 ps in 1,2-dichloroethane. The charge-shift state collapses, in part, back to the ground state but it also leads to partial triplet formation; the discrimination between rates for the forward and reverse processes is circa 7.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Chemistry & Advanced Materials, Materials Science and Environmental Engineering, Newcastle University, United Kingdom

Contributors: He, X., Benniston, A. C., Lemmetyinen, H., Tkachenko, N. V.

Pages: 277-282

Publication date: Mar 2018

Peer-reviewed: Yes

#### Publication information

Journal: ChemPhotoChem

Volume: 2

Issue number: 3

ISSN (Print): 2367-0932

Original language: English

DOIs:

10.1002/cptc.201700184

Research output: Contribution to journal > Article > Scientific > peer-review

#### Chemical Dissolution of Pt(111) During Potential Cycling Under Negative pH Conditions Studied by Operando X-ray Photoelectron Spectroscopy

Dissolution of platinum catalyst is a major degradation mechanism of fuel cells but the exact reaction mechanism has remained unclear. Here, electrochemical ambient pressure X-ray photoelectron spectroscopy (EC-APXPS) was utilized to provide direct information on chemical species on a single crystal Pt(111) electrode under extremely low pH conditions. Measurements were conducted using a novel condensed electrolyte film electrochemical cell applying work function measurement as a loss-free probe for electrochemical potential. We show that platinum can dissolve chemically as Pt<sup>2+</sup> ion during potential cycling and redeposit as Pt<sup>2+</sup> at the onset potential for cathodic reactions. The dissolution of Pt does not require electrochemical oxidation via oxide place-exchange. In contrast, the adsorption of oxygenated species (OH\* or O\*) at the onset potential for anodic reactions is a sufficient prerequisite to the dissolution. These results provide new insight to the degradation mechanism of Pt under extremely low pH conditions, predicted by the Pourbaix diagram, having practical applications to the durability of Pt-based catalysts in electrochemical energy conversion devices.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Research group: Surface Science, Stanford Synchrotron Radiation Light Source, SLAC National Accelerator Laboratory, Stockholm University

Contributors: Ali-Löyty, H., Valden, M., Hannula, M., Eilert, A., Ogasawara, H., Nilsson, A.

Pages: 25128-25134

Publication date: 25 Sep 2019

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry C

Volume: 123

Issue number: 41

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2019): CiteScore 7.3 SJR 1.477 SNIP 1.063

Original language: English

Electronic versions:

acs.jpcc.9b05201

DOIs:

10.1021/acs.jpcc.9b05201

URLs:

<http://urn.fi/URN:NBN:fi:tuni-201910244070>

Additional files:

#### Supporting information

Research output: Contribution to journal > Article > Scientific > peer-review

### Coating of Silica and Titania Aerosol Nanoparticles by Silver Vapor Condensation

Silica and titania aerosol nanoparticles are coated with silver through a physical coating process. The silver is evaporated in a tubular furnace flow system and condensed on the ceramic carrier particles with diameters of approximately 100nm. The temperature gradient in the furnace system is optimized in order to avoid homogeneous nucleation of the silver. The generated ceramic-silver composite nanoparticles are characterized with aerosol measurements and analytical transmission electron microscopy. Two completely different particle morphologies are clearly observed, silver-decoration and composite doublet, with amorphous silica and crystalline rutile titania as the carrier particles, respectively. The former morphology consists of multiple silver nanodots with diameters of 1-10nm, while in the latter morphology the silver had formed a larger structure with a size comparable to that of the carrier particle. Different shapes are observed in these larger silver structures, such as triangular, rodlike, and hexagonal. Differences in the silver particle migration on the surface of the silica and titania particles is proposed to be the key factor resulting into the two distinct particle morphologies. Copyright 2015 American Association for Aerosol Research

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Engineering materials science and solutions (EMASS), Department of Physics, Research area: Aerosol Physics, Research group: Aerosol Synthesis, Department of Materials Science, Research group: Materials Characterization

Contributors: Harra, J., Juuti, P., Haapanen, J., Sorvali, M., Roumeli, E., Honkanen, M., Vippola, M., Yli-Ojanperä, J., Mäkelä, J. M.

Number of pages: 10

Pages: 767-776

Publication date: 2 Sep 2015

Peer-reviewed: Yes

#### Publication information

Journal: Aerosol Science and Technology

Volume: 49

Issue number: 9

ISSN (Print): 0278-6826

Ratings:

Scopus rating (2015): CiteScore 4.5 SJR 1.309 SNIP 1.032

Original language: English

Keywords: LIQUID FLAME SPRAY, LOW-PRESSURE IMPACTOR, GAS-PHASE, PARTICLES, CATALYST, DEPOSITION, SIZE, ALUMINA, GROWTH, PARAMETERS

DOIs:

10.1080/02786826.2015.1072263

#### Bibliographical note

ORG=fys,0.5

ORG=mol,0.5

Source: WOS

Source ID: 000359160300002

Research output: Contribution to journal > Article > Scientific > peer-review

### Composite Hydrogels Using Bioinspired Approach with in Situ Fast Gelation and Self-Healing Ability as Future Injectable Biomaterial

Biopolymers are attractive candidates to fabricate biocompatible hydrogels, but the low water solubility of most of them at physiological pH has hindered their applications. To prepare a water-soluble derivative of chitosan (WSC) biopolymer, it was grafted with a small anionic amino acid, L-glutamic acid, using a single-step 1-ethyl-3-[3-dimethylaminopropyl]carbodiimide coupling reaction. This resulted in a zwitterion-tethered structure onto the polymer backbone. The degree of substitution range was  $13-16 \pm 1.25\%$ , which was controlled by varying the feeding reagent ratios. Differential scanning calorimetry- and X-ray diffraction-based analysis confirmed a transition from amorphous into a moderately amorphous/crystalline morphology after amino acid grafting, which made the derivative water-soluble at physiological pH. Composite hydrogels gelled within 60 s when using this WSC together with benzaldehyde-terminated 4-arm poly(ethylene glycol) as cross-linker. The compressive modulus of these hydrogels could be easily tuned between  $4.0 \pm 1.0$  and  $31 \pm 2.5$  kPa, either by changing the cross-linker concentration or total solid content in the final gel. The gels were injectable at the lowest cross-linker as well as total solid content, due to the enhanced elastic behavior. These hydrogels showed biodegradability during a 1 month incubation period in phosphate-buffered saline with weight remaining of  $60 \pm 1.5$  and  $44 \pm 1.45\%$  at pHs 7.4 and 6.5, respectively. The cytocompatibility of the gels was tested using the fibroblast cell line (i.e., WI-38), which showed good cell viability on the gel surface. Therefore, these hydrogels could be an important injectable biomaterial for delivery purpose in the future.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Faculty of Biomedical Sciences and Engineering, Chemistry and Bioengineering, Materials Science, Research group: Biomaterials and Tissue Engineering Group, BioMediTech, Institute of Chemical Sciences, 25120 Peshawar, Pakistan

Contributors: Khan, M., Koivisto, J., Hukka, T., Hokka, M., Kellomäki, M.

Pages: 11950-11960

Publication date: 11 Apr 2018

Peer-reviewed: Yes

Early online date: 15 Mar 2018

### Publication information

Journal: ACS Applied Materials & Interfaces

Volume: 10

Issue number: 14

ISSN (Print): 1944-8244

Ratings:

Scopus rating (2018): CiteScore 12.4 SJR 2.596 SNIP 1.559

Original language: English

ASJC Scopus subject areas: Materials Science(all), Chemistry(all)

DOIs:

10.1021/acsami.8b01351

Research output: Contribution to journal > Article > Scientific > peer-review

### Convenient extraction method for quantification of thin zinc patina layers

Synthetic zinc patina was grown on galvanized steel sheets in supercritical carbon dioxide atmosphere. Different patina compounds were dissolved and quantified using a stepwise immersion and dissolution procedure. The distinct patina components, namely anhydrous zinc carbonate (a dense layer adjacent to metallic zinc) and zinc hydroxy carbonate (nanowires on the surface), were dissolved in glycine solutions, followed by quantification of  $Zn^{2+}$  in the solutes by X-ray fluorescence. The zinc hydroxy carbonate nanowires were readily glycine soluble, and the anhydrous zinc carbonate showed scarce glycine solubility, which enabled their selective quantification. The amount of the remaining (anhydrous) zinc carbonate after glycine extraction was determined from the glycine-soluble zinc oxide after calcination (heat treatment for 10 minutes at 350°C). The results were verified by scanning electron microscopy imaging and Fourier transform infrared spectroscopy measurements.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science

Contributors: Saarimaa, V., Kaleva, A., Paunikallio, T., Nikkanen, J., Heinonen, S., Levänen, E., Väisänen, P., Markkula, A.

Pages: 564-570

Publication date: 2018

Peer-reviewed: Yes

Early online date: 1 Jan 2018

### Publication information

Journal: Surface and Interface Analysis

Volume: 50

Issue number: 5

ISSN (Print): 0142-2421

Ratings:

Scopus rating (2018): CiteScore 2.4 SJR 0.451 SNIP 0.648

Original language: English

ASJC Scopus subject areas: Chemistry(all), Condensed Matter Physics, Surfaces and Interfaces, Surfaces, Coatings and Films, Materials Chemistry

Keywords: Galvanized steel, Glycine, Supercritical carbon dioxide, Zinc carbonate, Zinc nanowires, Zinc oxide

DOIs:

10.1002/sia.6429

Source: Scopus

Source ID: 85044219012

Research output: Contribution to journal > Article > Scientific > peer-review

### **Corrosion products of carbonation induced corrosion in existing reinforced concrete facades**

Active corrosion in reinforced concrete structures is controlled by environmental conditions and material properties. These factors determine the corrosion rate and type of corrosion products which govern the total achieved service life. The type and critical amount of corrosion products were studied by electron microscopy and X-ray diffractometry on concrete and reinforcement samples from existing concrete facades on visually damaged locations. The corrosion products in outdoor environment exposed concrete facades are mostly hydroxides (Feroxyhite, Goethite and Lepidocrocite) with a volume ratio to Fe of approximately 3. The results can be used to calibrate calculation of the critical corrosion penetration of concrete facade panels.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Civil Engineering, Research group: Service Life Engineering of Structures, Department of Materials Science, Research group: Materials Characterization, Research area: Structural Engineering, Engineering materials science and solutions (EMASS), Life Cycle Effectiveness of the Built Environment (LCE@BE)

Contributors: Köliö, A., Honkanen, M., Lahdensivu, J., Vippola, M., Pentti, M.

Number of pages: 8

Pages: 200-207

Publication date: Dec 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Cement and Concrete Research

Volume: 78

ISSN (Print): 0008-8846

Ratings:

Scopus rating (2015): CiteScore 6.4 SJR 3.549 SNIP 3.152

Original language: English

ASJC Scopus subject areas: Materials Science(all), Building and Construction

Keywords: B. SEM, B. X-ray diffraction, C. Corrosion, D. Reinforcement, E. Concrete

DOIs:

10.1016/j.cemconres.2015.07.009

URLs:

<http://www.scopus.com/inward/record.url?scp=84939174724&partnerID=8YFLogxK> (Link to publication in Scopus)

#### **Bibliographical note**

ORG=rak,0.75

ORG=mol,0.25

Source: Scopus

Source ID: 84942989347

Research output: Contribution to journal › Article › Scientific › peer-review

### **Cracking resistance of Cr<sub>3</sub>C<sub>2</sub>-NiCr and WC-Cr<sub>3</sub>C<sub>2</sub>-Ni thermally sprayed coatings under tensile bending stress**

The cracking behaviour of Cr<sub>3</sub>C<sub>2</sub>-25(Ni<sub>20</sub>Cr) and WC-20Cr<sub>3</sub>C<sub>2</sub>-7Ni thermally sprayed coatings during tensile load in 3-point bending tests was studied by Acoustic Emission (AE) monitoring and microstructure post-analysis. The AE monitoring reveals a superior resistance against cracking in the WC-Cr<sub>3</sub>C<sub>2</sub>-Ni coatings compared to Cr<sub>3</sub>C<sub>2</sub>-NiCr. The incorporation of tungsten carbides beneficially affects the residual stress state of the coatings and has an impact on the detailed fracture mode. The results hold for both as-sprayed as well as ground and polished coatings.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science

Contributors: Mayrhofer, E., Janka, L., Mayr, W. P., Norpoth, J., Rodriguez Ripoll, M., Gröschl, M.

Number of pages: 7

Pages: 169-175

Publication date: 15 Nov 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Surface and Coatings Technology

Volume: 281

ISSN (Print): 0257-8972

Ratings:

Scopus rating (2015): CiteScore 3.9 SJR 0.852 SNIP 1.376

Original language: English

Keywords: Acoustic emission, HVOF thermal spray coating, Cr3C2, WC, Bending test, Cracking

DOIs:

10.1016/j.surfcoat.2015.09.002

URLs:

<http://www.sciencedirect.com/science/article/pii/S0257897215302401>

Source: RIS

Source ID: urn:491ED12C7B5035BD6279AED841362E4F

Research output: Contribution to journal › Article › Scientific › peer-review

## Creation of superhydrophilic surfaces of paper and board

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Energy and Process Engineering, Department of Physics, Engineering materials science and solutions (EMASS)

Contributors: Tuominen, M., Teisala, H., Aromaa, M., Stepien, M., Mäkelä, J. M., Saarinen, J. J., Toivakka, M., Kuusipalo, J.

Pages: 864-879

Publication date: 2014

Peer-reviewed: Yes

### Publication information

Journal: Journal of Adhesion Science and Technology

Volume: 28

Issue number: 8-9

ISSN (Print): 0169-4243

Ratings:

Scopus rating (2014): CiteScore 2 SJR 0.398 SNIP 0.65

Original language: English

DOIs:

10.1080/01694243.2012.697744

URLs:

<http://www.tandfonline.com>

### Bibliographical note

Version of record first published: 13 Aug 2012. Ei UT-numeroa 30.8.2013 : Poistettu tupla r=1324

portfolio13<br/>Contribution: organisation=epr,FACT1=0.5<br/>Contribution: organisation=fys,FACT2=0.5<br/>Publisher

name: Taylor & Francis Group

Source: researchoutputwizard

Source ID: 1654

Research output: Contribution to journal › Article › Scientific › peer-review

## Digital imaging measurement of dense multiphase flows in industrial processes

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Energy and Process Engineering

Contributors: Honkanen, M., Eloranta, H., Saarenrinne, P.

Pages: 25-32

Publication date: 2010

Peer-reviewed: Yes

### Publication information

Journal: Flow Measurement and Instrumentation

Volume: 21

Issue number: 1

ISSN (Print): 0955-5986

Ratings:



Scopus rating (2010): SJR 0.572 SNIP 1.613

Original language: English

DOIs:

10.1016/j.flowmeasinst.2009.11.001

#### Bibliographical note

Contribution: organisation=epr,FACT1=1

Source: researchoutputwizard

Source ID: 8093

Research output: Contribution to journal › Article › Scientific › peer-review

#### Dissolution of enzyme-treated cellulose using freezing thawing method and the properties of fibres regenerated from the solution

The rapid coagulation of NaOH-based cellulose solution during the wet spinning process leads to a low stretching ratio and, consequently, the low mechanical properties of the fibres. The aim of this work was to slow down the coagulation by replacing the sulphuric acid spin bath with an acetic acid bath. The spin dope was prepared by dissolving the enzyme-treated dissolving pulp in aqueous sodium zincate using a freezing thawing method. The optimal zinc oxide and sodium hydroxide concentrations were studied first. The most thermally stable cellulose solution contained 6.5 wt% NaOH and 1.3 wt% ZnO with 6 wt% enzyme-treated dissolving pulp. The spin dope was prepared accordingly. Coagulation of the cellulose solution slowed down in the acetic acid bath, resulting in a significantly higher stretching ratio for the fibres than with the sulphuric acid bath. However, the acetic acid spun fibres shrunk strongly during drying, and the possibly aligned order of the molecular chains due to the high stretch was partly lost. As a consequence, the high stretch was not transferred to high tenacity of the fibres in this study. However, the result suggests attractive potential to develop processing conditions to increase fibre tenacity.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Fibre Materials, Research group: Materials Characterization, Engineering materials science and solutions (EMASS), VTT Tech Res Ctr Finland, VTT Technical Research Center Finland, Aalto Univ, Aalto University, Sch Chem Technol, Dept Forest Prod Technol

Contributors: Vehviläinen, M., Kamppuri, T., Gronqvist, S., Rissanen, M., Maloney, T., Honkanen, M., Nousiainen, P.

Number of pages: 22

Pages: 1653-1674

Publication date: Jun 2015

Peer-reviewed: Yes

#### Publication information

Journal: Cellulose

Volume: 22

Issue number: 3

ISSN (Print): 0969-0239

Ratings:

Scopus rating (2015): CiteScore 5.2 SJR 1.122 SNIP 1.202

Original language: English

Keywords: Cellulose dissolution, Dissolving pulp, Enzymatic treatment, Wet spinning, Regenerated fibres, Biocelsol, NAOH/UREA AQUEOUS-SOLUTION, SODIUM-HYDROXIDE, DISSOLVING PULP, WET-SPUN, TEMPERATURE, MULTIFILAMENT, CARBAMATE, MECHANISM, SYSTEM

DOIs:

10.1007/s10570-015-0632-0

Source: WOS

Source ID: 000354193000015

Research output: Contribution to journal › Article › Scientific › peer-review

#### Economic analysis of hydrogen production by methane thermal decomposition: Comparison to competing technologies

This study is a comparative analysis of hydrogen production costs in current and potential future market environments. The economic feasibility of hydrogen production by thermal decomposition of methane was compared to two other technologies, namely steam methane reforming and water electrolysis. According to the results, thermal decomposition of methane would be most suited for on-site demand-driven hydrogen production in small or medium industrial scale. Hydrogen production by thermal decomposition of methane would be economically competitive with steam reforming with a product carbon value of at least 280-310 EUR/tonne. By contrast, the main benefit of thermal decomposition of methane in comparison with water electrolysis is the feedstock availability via the current natural gas infrastructure, whereas electrolysis is highly dependent on the cost and availability of renewable electricity. The major factors affecting the economic feasibility were identified as product carbon value in thermal decomposition of methane, natural gas cost in steam reforming, and electricity cost in electrolysis. Thus, the effect of these variables on the hydrogen production costs

was analyzed. Additionally, the specific carbon dioxide emissions in hydrogen production by thermal decomposition of methane (40 kgCO<sub>2</sub>/MWhH<sub>2</sub>) were found to be much less than that by steam reforming coupled with carbon dioxide capture from the syngas (133 kgCO<sub>2</sub>/MWhH<sub>2</sub>).

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy  
Contributors: Keipi, T., Tolvanen, H., Kontinen, J.  
Number of pages: 10  
Pages: 264-273  
Publication date: 1 Mar 2018  
Peer-reviewed: Yes

#### Publication information

Journal: Energy Conversion and Management  
Volume: 159  
ISSN (Print): 0196-8904  
Ratings:  
Scopus rating (2018): CiteScore 12.4 SJR 2.73 SNIP 2.181  
Original language: English  
Keywords: Methane decomposition, hydrogen, economic analysis, carbon dioxide emissions  
DOIs:  
10.1016/j.enconman.2017.12.063  
Research output: Contribution to journal › Article › Scientific › peer-review

#### Effect of alkali and silane surface treatments on regenerated cellulose fibre type (Lyocell) intended for composites

Cellulose fibres have significant importance and potential for polymer reinforcement. It is essential to modify the surface of the fibre to obtain good fibre-matrix interface. Surface treatments can increase surface roughness of the fibre, change its chemical composition and introduce new moieties that can effectively interlock with the matrix, resulting in good mechanical properties in the composites. This is mainly due to improved fibre-matrix adhesion. The treatments may also reduce the water absorption rate by converting part of the hydroxyl groups on the fibre surface into other functional groups. Chemical modification of the surface of a regenerated cellulose fibre of the Lyocell type was carried out by alkali and silane treatments, which significantly changed the properties of the Lyocell fibres. Three parameters were considered when the fibre surface treatment was done: concentration (2–15 wt%), temperature (25 and 50 °C) and time (30 min–72 h). Fourier transform infrared spectroscopy and Raman spectroscopy were used for chemical analysis and qualitative analysis of the cellulose crystallinity due to the surface treatments; subsequently, mechanical strength of the fibres was tested by tensile testing. Weight loss, moisture regain and swelling measurements were taken before and after treatments, which showed the obvious changes in fibre properties on treatment. Heat capacity of the fibres was measured for untreated and treated fibres, and thermal degradation of fibres was examined to see the stability of fibres at elevated temperatures. Wettability and surface energies were measured using dynamic contact angle method in three wetting mediums. Scanning electron microscopy was used to study the morphological properties of the fibres.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Department of Materials Science, Research group: Fibre Materials, University College of Borås, Högskolan i Borås, Swedish Centre for Resource Recovery  
Contributors: Ramamoorthy, S. K., Skrifvars, M., Rissanen, M.  
Number of pages: 18  
Pages: 637-654  
Publication date: 2015  
Peer-reviewed: Yes

#### Publication information

Journal: Cellulose  
Volume: 22  
Issue number: 1  
ISSN (Print): 0969-0239  
Ratings:  
Scopus rating (2015): CiteScore 5.2 SJR 1.122 SNIP 1.202  
Original language: English  
ASJC Scopus subject areas: Polymers and Plastics  
Keywords: Alkali, Cellulose, Fibre, Lyocell, Silane, Surface modification  
DOIs:

10.1007/s10570-014-0526-6

URLs:

<http://www.scopus.com/inward/record.url?scp=84921943065&partnerID=8YFLogxK> (Link to publication in Scopus)

#### **Bibliographical note**

EXT="Skrifvars, Mikael"

Source: Scopus

Source ID: 84921943065

Research output: Contribution to journal › Article › Scientific › peer-review

### **Effect of fibre properties on flocculation and fractionation of cellulosic fibres in dry state**

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Energy and Process Engineering

Contributors: Larkomaa, J., Niinimäki, J., Honkanen, M., Hanif, M., Saarenrinne, P.

Number of pages: 10

Pages: 1-10

Publication date: 2010

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Engineered Fibers and Fabrics

Volume: 5

Issue number: 1

ISSN (Print): 1558-9250

Ratings:

Scopus rating (2010): SJR 0.171 SNIP 0.284

Original language: English

URLs:

<http://www.jeffjournal.org>

#### **Bibliographical note**

Contribution: organisation=epr,FACT1=1

Source: researchoutputwizard

Source ID: 8582

Research output: Contribution to journal › Article › Scientific › peer-review

### **Effect of rheological properties of dissolved cellulose/microfibrillated cellulose blend suspensions on film forming**

Enzymatically treated cellulose was dissolved in a NaOH/ZnO solvent system and mixed together with microfibrillated cellulose (MFC) in order to find the threshold in which MFC fibers form a percolation network within the dissolved cellulose solution and in order to improve the properties of regenerated cellulose films. In the aqueous state, correlations between the rheological properties of dissolved cellulose/MFC blend suspensions and MFC fiber concentrations were investigated and rationalized. In addition, rheological properties of diluted MFC suspensions were characterized and a correlation with NaOH concentration was found, thus partly explaining the flow properties of dissolved cellulose/MFC blend suspensions. Finally, based on results from Dynamic Mechanical Analysis (DMA), MFC addition had strengthening/plasticizing effect on regenerated cellulose films if low concentrations of MFC, below the percolation threshold (5.5-6 wt%, corresponding to 0.16-0.18 wt% of MFC in the blend suspensions), were used.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Fibre Materials, PolymerTechnology, Department of Biotechnology and Chemical Technology, Aalto University

Contributors: Saarikoski, E., Rissanen, M., Seppälä, J.

Number of pages: 9

Pages: 62-70

Publication date: 30 Mar 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Carbohydrate Polymers

Volume: 119

ISSN (Print): 0144-8617

Ratings:

Scopus rating (2015): CiteScore 7.8 SJR 1.44 SNIP 1.82

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Materials Chemistry, Polymers and Plastics

Keywords: Blend, Dissolved cellulose, Microfibrillated cellulose, Rheology, Suspension

DOIs:

10.1016/j.carbpol.2014.11.033

URLs:

<http://www.scopus.com/inward/record.url?scp=84916613635&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84916613635

Research output: Contribution to journal > Article > Scientific > peer-review

## Effects of flame and corona treatment on extrusion coated paper properties

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Energy and Process Engineering, Engineering materials science and solutions (EMASS)

Contributors: Tuominen, M., Lahti, J., Kuusipalo, J.

Pages: 29-36

Publication date: 2011

Peer-reviewed: Yes

### Publication information

Journal: TAPPI Journal

Volume: 10

Issue number: 10

ISSN (Print): 0734-1415

Ratings:

Scopus rating (2011): SJR 0.592 SNIP 1.101

Original language: English

### Bibliographical note

Contribution: organisation=epr pap,FACT1=1

Source: researchoutputwizard

Source ID: 7422

Research output: Contribution to journal > Article > Scientific > peer-review

## Electronically Coupled Uranium and Iron Oxide Heterojunctions as Efficient Water Oxidation Catalysts

The most critical challenge faced in realizing a high efficiency photoelectrochemical water splitting process is the lack of suitable photoanodes enabling the transfer of four electrons involved in the complex oxygen evolution reaction (OER). Uranium oxides are efficient catalysts due to their wide range optical absorption (E-g approximate to 1.8-3.2 eV), high photoconductivity, and multiple valence switching among uranium centers that improves the charge propagation kinetics. Herein, thin films of depleted uranium oxide (U<sub>3</sub>O<sub>8</sub>) are demonstrated grown via chemical vapor deposition effectively accelerate the OER in conjunction with hematite (alpha-Fe<sub>2</sub>O<sub>3</sub>) overlayers through a built-in potential at the interface. Density functional theory simulations demonstrate that the multivalence of U and Fe ions induce the adjustment of the band alignment subject to the concentration of interfacial Fe ions. In general, the equilibrium state depicts a type II band edge as the favored alignment, which improves charge-transfer processes as observed in transient and X-ray absorption (TAS and XAS) spectroscopy. The enhanced water splitting photocurrent density of the heterostructures (J = 2.42 mA cm<sup>-2</sup>) demonstrates the unexplored potential of uranium oxide in artificial photosynthesis.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Research group: Chemistry & Advanced Materials

Contributors: Leduc, J., Gönüllü, Y., Ruoko, T., Fischer, T., Mayrhofer, L., Tkachenko, N. V., Dong, C., Held, A., Moseler, M., Mathur, S.

Number of pages: 7

Publication date: 3 Oct 2019

Peer-reviewed: Yes

### Publication information

Journal: Advanced Functional Materials

Article number: 1905005

ISSN (Print): 1616-301X

Ratings:

Scopus rating (2019): CiteScore 22 SJR 5.875 SNIP 2.45

Original language: English

Keywords: absorption spectroscopy, DFT simulations, heterojunction, OER, photoelectrochemical water splitting, ULTRATHIN HEMATITE FILMS, LAYER-BY-LAYER, THIN-FILM, TRANSITION-METAL, OXYGEN, STATES, EVOLUTION, SPECTROSCOPY, PERFORMANCE, UNDERLAYER

Electronic versions:

Electronically Coupled Uranium and Iron Oxide 2019

DOIs:

10.1002/adfm.201905005

URLs:

<http://urn.fi/URN:NBN:fi:tuni-202003032485>

Source: WOS

Source ID: 000491124400001

Research output: Contribution to journal > Article > Scientific > peer-review

### **Electronic couplings and rates of excited state charge transfer processes at poly(thiophene-co-quinoxaline)-PC<sub>71</sub>BM interfaces: two- versus multi-state treatments**

Electronic coupling between adjacent molecules is one of the key parameters determining the charge transfer (CT) rates in bulk heterojunction (BHJ) polymer solar cells (PSCs). We calculate theoretically electronic couplings for exciton dissociation (ED) and charge recombination (CR) processes at local poly(thiophene-co-quinoxaline) (TQ)-PC<sub>71</sub>BM interfaces. We use eigenstate-based coupling schemes, i.e. the generalized Mulliken-Hush (GMH) and fragment charge difference (FCD) schemes, including 2 to multiple (3–11) states. Moreover, we study the effects of functionals, excited state methods, basis sets, surrounding media, and relative placements of TQ and PC<sub>71</sub>BM on the coupling values. Generally, both schemes provide consistent couplings with the global hybrid functionals, which yield more charge-localized diabatic states and constant coupling values regardless of the number of states, and so the 2-state schemes may be sufficient. The (non-tuned and optimally tuned) long-range corrected (LRC) functionals result in more notable mixing of the local components with the CT states. Employing multiple states reduces the mixing and thus improves the LRC results, although the method still affects the GMH CR couplings. As the FCD scheme is less sensitive, we recommend combining it with the multi-state treatment for polymer-fullerene systems when using the LRC functionals. Finally, we employ the 11-state FCD couplings to calculate the ED and CR rates, which are consistent with the experimental rates of the polymer-fullerene systems. Our results provide more insight into choosing a suitable eigenstate-based coupling scheme for predicting the electronic couplings and CT rates in photoactive systems.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Research group: Chemistry & Advanced Materials, Computing Sciences, Physics, Linköping University, University of Brasilia

Contributors: Kastinen, T., da Silva Filho, D. A., Paunonen, L., Linares, M., Ribeiro Junior, L. A., Cramariuc, O., Hukka, T. I.

Number of pages: 20

Pages: 25606-25625

Publication date: 1 Nov 2019

Peer-reviewed: Yes

#### **Publication information**

Journal: Physical Chemistry Chemical Physics

Volume: 21

Issue number: 46

ISSN (Print): 1463-9076

Ratings:

Scopus rating (2019): CiteScore 6.3 SJR 1.143 SNIP 0.98

Original language: English

Electronic versions:

Electronic couplings and rates of excited state charge transfer processes

DOIs:

10.1039/C9CP04837E

URLs:

<http://urn.fi/URN:NBN:fi:tuni-201912136875>

Additional files:

ESI\_PCCP\_Kastinen\_Hukka\_etal

Source: Bibtex

Source ID: C9CP04837E

Research output: Contribution to journal > Article > Scientific > peer-review

### **Electrospun Black Titania Nanofibers: Influence of Hydrogen Plasma-Induced Disorder on the Electronic Structure and Photoelectrochemical Performance**

This work encompasses a facile method for tailoring surface defects in electrospun TiO<sub>2</sub> nanofibers by employing hydrogen plasma treatments. This amiable processing method was proven with SQUID, EPR, and XPS to be highly effective in generating oxygen vacancies, accompanied by the reduction of Ti<sup>4+</sup> centers to Ti<sup>3+</sup>, resulting in the formation of black titania. The treatment temperature was found to affect the Ti<sup>3+</sup>/Ti<sup>4+</sup> ratios and surface valence, while preserving the original 1D morphology of the titania fibers. Ab initio DFT calculations showed that a high concentration of oxygen vacancies is highly efficient in producing midgap states that enhance the system absorption over the whole visible range, as observed with UV/vis/NIR diffuse reflectance spectroscopy. Pristine TiO<sub>2</sub> nanofibers produced a photocurrent density of similar to 0.02 mA/cm<sup>2</sup> at 1.23 V vs RHE, whereas the hydrogen plasma treatment resulted in up to a 10-fold increase in the photoelectrochemical performance.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Università degli Studi di Padova, Italy, Univ Cologne, University of Cologne, Dept Chem, Chair Inorgan & Mat Chem, Padova University, INSTM, J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Institute of Inorganic Chemistry, Catalonia Institute for Energy Research (IREC), Multiscale Materials Modelling and Tribo Simulation, CNR-IENI

Contributors: Lepcha, A., Maccato, C., Mettenbörger, A., Andreu, T., Mayrhofer, L., Walter, M., Olthof, S., Ruoko, T. P., Klein, A., Moseler, M., Meerholz, K., Morante, J. R., Barreca, D., Mathur, S.

Number of pages: 8

Pages: 18835-18842

Publication date: 20 Aug 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Journal of Physical Chemistry C

Volume: 119

Issue number: 33

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2015): CiteScore 7.9 SJR 1.886 SNIP 1.246

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)

Keywords: ROOM-TEMPERATURE, WATER, SURFACE, NANOSTRUCTURES, NANOPARTICLES, PHOTOCATALYSIS, INSULATORS, CONVERSION, DEFECTS, ARRAYS

Electronic versions:

Electrospun\_black\_titania\_nanofibers\_post-print

DOIs:

10.1021/acs.jpcc.5b02767

URLs:

<http://urn.fi/URN:NBN:fi:tty-201612094845>

URLs:

<http://www.scopus.com/inward/record.url?scp=84939825598&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84939825598

Research output: Contribution to journal > Article > Scientific > peer-review

### **Engineering and Characterization of Bacterial Nanocellulose Films as Low Cost and Flexible Sensor Material**

Some bacterial strains such as *Komagataeibacter xylinus* are able to produce cellulose as an extracellular matrix. In comparison to wood-based cellulose, bacterial cellulose (BC) holds interesting properties such as biodegradability, high purity, water-holding capacity, and superior mechanical and structural properties. Aiming toward improvement in BC production titer and tailored alterations to the BC film, we engineered *K. xylinus* to overexpress partial and complete bacterial cellulose synthase operon that encodes activities for BC production. The changes in cell growth, end metabolite, and BC production titers from the engineered strains were compared with the wild-type *K. xylinus*. Although there were no

significant differences between the growth of wild-type and engineered strains, the engineered *K. xylinus* strains demonstrated faster BC production, generating 2–4-fold higher production titer (the highest observed titer was obtained with *K. xylinus*-bcsABCD strain producing  $4.3 \pm 0.46$  g/L BC in 4 days). The mechanical and structural characteristics of cellulose produced from the wild-type and engineered *K. xylinus* strains were analyzed with a stylus profilometer, in-house built tensile strength measurement system, a scanning electron microscope, and an X-ray diffractometer. Results from the profilometer indicated that the engineered *K. xylinus* strains produced thicker BC films (wild type, 5.1  $\mu\text{m}$ , and engineered *K. xylinus* strains, 6.2–10.2  $\mu\text{m}$ ). Scanning electron microscope revealed no principal differences in the structure of the different type BC films. The crystallinity index of all films was high (from 88.6 to 97.5%). All BC films showed significant piezoelectric response (5.0–20 pC/N), indicating BC as a promising sensor material.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: BioMediTech, Chemistry and Bioengineering, Faculty of Biomedical Sciences and Engineering, Materials Science, Research group: Plastics and Elastomer Technology, Research group: Plastics and Elastomer Technology, Research group: Industrial Bioengineering and Applied Organic Chemistry, Research group: Bio- and Circular Economy, Research area: Microsystems, Research area: Measurement Technology and Process Control, Research group: Sensor Technology and Biomeasurements (STB)

Contributors: Mangayil, R., Rajala, S., Pammo, A., Sarlin, E., Luo, J., Santala, V., Karp, M., Tuukkanen, S.

Number of pages: 9

Pages: 19048–19056

Publication date: 2017

Peer-reviewed: Yes

Early online date: 18 May 2017

### Publication information

Journal: ACS Applied Materials & Interfaces

Volume: 9

Issue number: 22

ISSN (Print): 1944-8244

Ratings:

Scopus rating (2017): CiteScore 11.3 SJR 2.784 SNIP 1.543

Original language: English

Electronic versions:

Mangayil\_2017\_Bacterial\_cellulose\_pietzo\_Postprint. Embargo ended: 18/05/18

DOIs:

10.1021/acsami.7b04927

URLs:

<http://urn.fi/URN:NBN:fi:tyy-201802151246>. Embargo ended: 18/05/18

Source: RIS

Source ID: urn:9654BBA35A6BF054571845C06F06F5D9

Research output: Contribution to journal > Article > Scientific > peer-review

### Enhanced pre-treatment of cellulose pulp prior to dissolution into NaOH/ZnO

As a result of the constantly growing demand for textile fibres interest in utilising cellulose pulps for manufacturing regenerated cellulose fibres is growing. One promising water-based process for the manufacture of regenerated cellulosic products is the Biocelsol process based on an NaOH/ZnO solvent system. The drawback of the Biocelsol process is the need for pre-treatment of the pulp, i.e. long mechanical pre-treatment (up to 5 h) followed by a 2–3-h enzymatic hydrolysis utilising a rather high amount of cellulolytic enzymes. In this work more efficient conditions to carry out the pre-treatment of cellulose pulp prior to dissolution into NaOH/ZnO are presented. Based on the results, cellulase treatment, when carried out in an extruder, can be used to effectively open up and fibrillate the fibres without completely destroying the fibre structure. The molar mass of the pulp treated enzymatically in an extruder was 14 % lower as compared to the state-of-the-art-treated cellulose. As a consequence, the alkaline solutions prepared from the pulp treated enzymatically in an extruder had clearly lower dope viscosities regarding the cellulose content than the solutions prepared from the state-of-the-art-treated pulp. This enabled increasing the cellulose content in the dope up to 7 % (w/w) without increasing the dope viscosity.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Fibre Materials, Department of Forest Products Technology, VTT Technical Research Centre of Finland, Aalto University

Contributors: Grönqvist, S., Kamppuri, T., Maloney, T., Vehviläinen, M., Liittä, T., Suurnäkki, A.

Number of pages: 10

Pages: 3981-3990

Publication date: Dec 2015

Peer-reviewed: Yes

### Publication information

Journal: Cellulose

Volume: 22

Issue number: 6

ISSN (Print): 0969-0239

Ratings:

Scopus rating (2015): CiteScore 5.2 SJR 1.122 SNIP 1.202

Original language: English

ASJC Scopus subject areas: Polymers and Plastics

Keywords: Biocelsol, Cellulose dissolution, Dissolving pulp, Enzymatic hydrolysis, Porosity, Pre-treatment, Solute exclusion

DOIs:

10.1007/s10570-015-0742-8

URLs:

<http://www.scopus.com/inward/record.url?scp=84942026378&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84946493808

Research output: Contribution to journal › Article › Scientific › peer-review

### Enhancing piezoelectric properties of bacterial cellulose films by incorporation of MnFe<sub>2</sub>O<sub>4</sub> nanoparticles

Low-cost and highly sensitive piezoelectric sensors were fabricated from bacterial cellulose (BC)/MnFe<sub>2</sub>O<sub>4</sub> nanocomposite films via a co-precipitation method, followed by hot-pressing. MnFe<sub>2</sub>O<sub>4</sub> nanoparticles were homogeneously distributed in the BC structure. The piezoelectric sensitivity measurements in the normal mode showed that the pristine BC film exhibited a sensitivity of ~5 pC/N, whereas this value was increased to 23 pC/N for the composite film, which is comparable to the PVDF reference film. In the bending mode, the piezoelectric response increased to 25 pC/N and 57 pC/N for the BC film and the composite film, respectively. Moreover, the piezoelectric sensitivity was significantly enhanced using carbon tape electrodes attached directly to the films instead of sandwiched electrodes. This produced a sensitivity of greater than 50 pC/N for the MBC nanocomposite film in the normal mode measurement. Our work demonstrates the potential of using MBC composite films as inexpensive and highly sensitive flexible piezoelectric sensors.

### General information

Publication status: E-pub ahead of print

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Research group: Bio- and Circular Economy, BioMediTech, Research group: Nanoscale Phenomena and Measurements (NPM), Research group: Sensor Technology and Biomeasurements (STB)

Contributors: Sriplai, N., Mangayil, R., Pammo, A., Santala, V., Tuukkanen, S., Pinitsoontorn, S.

Publication date: 10 Dec 2019

Peer-reviewed: Yes

### Publication information

Journal: Carbohydrate Polymers

Volume: 231

ISSN (Print): 0144-8617

Ratings:

Scopus rating (2019): CiteScore 11.7 SJR 1.514 SNIP 1.946

Original language: English

Keywords: Bacterial cellulose, Piezoelectric, Sensor, Composite, MnFeO

Electronic versions:

Enhancing Piezoelectric Properties 2019. Embargo ended: 10/12/20

DOIs:

10.1016/j.carbpol.2019.115730

URLs:

<http://urn.fi/URN:NBN:fi:tuni-202002031761>. Embargo ended: 10/12/20

Additional files:

Enhancing Piezoelectric Properties 2019\_Supplementary Information

Source: RIS

Source ID: urn:9C09FE8271D4B0D19A505EC77DF2EF4A

Research output: Contribution to journal › Article › Scientific › peer-review



## Entrapped Styrene Butadiene Polymer Chains by Sol-Gel-Derived Silica Nanoparticles with Hierarchical Raspberry Structures

A sol-gel transformation of liquid silica precursor to solid silica particles was carried out in a one-pot synthesis way, where a solution of styrene butadiene elastomer was present. The composites, thus produced, offered remarkable improvements of mechanical and dynamic mechanical performances compared to precipitated silica. The morphological analysis reveals that the alkoxy-based silica particles resemble a raspberry structure when the synthesis of the silica was carried out in the presence of polymer molecules and represent a much more open silica-network structure. However, in the absence of the polymer, the morphology of the silica particles is found to be different. It is envisaged that the special morphology of the in situ synthesized silica particles contributes to the superior reinforcement effects, which are associated with a strong silica-rubber interaction by rubber chains trapped inside the raspberry-like silica aggregates. Therefore, the interfaces are characterized in detail by low-field solid-state  $^1\text{H}$  NMR spectroscopy,  $^{29}\text{Si}$  solid-state NMR spectroscopy, and energy-dispersive X-ray spectroscopy. Low-field  $^1\text{H}$  NMR-based double-quantum experiments provide a quantitative information about the cross-link density of the silica-filled rubber composites and about the influence of silane coupling agent on the chemical cross-link density of the network and correlates well with equilibrium swelling measurements. The special microstructure of the alkoxy-based silica was found to be associated with the interaction between alkoxy-based silica and rubber chains as a consequence of particle growth in the presence of rubber chains.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Leibniz-Institut für Polymerforschung Dresden E.V., Vodafone Department of Mobile Communications Systems, Martin-Luther-Universität Halle-Wittenberg

Contributors: Vaikuntam, S. R., Stöckelhuber, K. W., Subramani Bhagavatheswaran, E., Wießner, S., Scheler, U., Saalwächter, K., Formanek, P., Heinrich, G., Das, A.

Number of pages: 13

Pages: 2010-2022

Publication date: 15 Feb 2018

Peer-reviewed: Yes

### Publication information

Journal: Journal of Physical Chemistry B

Volume: 122

Issue number: 6

ISSN (Print): 1520-6106

Ratings:

Scopus rating (2018): CiteScore 5.8 SJR 1.109 SNIP 0.979

Original language: English

ASJC Scopus subject areas: Physical and Theoretical Chemistry, Surfaces, Coatings and Films, Materials Chemistry  
DOIs:

10.1021/acs.jpcc.7b11792

Source: Scopus

Source ID: 85042152539

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

## Fermentative metabolism of an anaerobic, thermophilic consortium on plant polymers and commercial paper samples

The purpose of the study was to examine the feasibility and capacity of a thermophilic microbial consortium to produce fermentative metabolites from plant polymers. The consortium comprised of cellulolytic anaerobes that were originally enriched from a compost pile using cellulose as the substrate. Fermentative metabolism was examined with monosaccharides, disaccharides, hemicellulose, starch, pectin, chitin, and eight commercial paper samples without further enrichment of the culture to each specific substrate. In general,  $\text{H}_2$ ,  $\text{CH}_4$ ,  $\text{CO}_2$ , and organic acids were the main metabolites on all substrates but the metabolite profiles varied with the substrate. Similar  $\text{H}_2$  yields of  $2\text{--}3\text{molmol}^{-1}$  substrate at 48h were obtained with all monosaccharides and disaccharides. The  $\text{CO}_2$  yields were higher with disaccharides than with monosaccharides,  $4.5$  vs  $2\text{molmol}^{-1}$  substrate. Metabolite yields were relatively low with glyceraldehyde, glycerol, and arabinose. Paper samples containing high amounts of chemical pulp produced the highest metabolite yields, and biodegradation accounted for  $\leq 74\%$  of total dry weight loss. The fermentative metabolism of the paper samples varied with the pulp composition and the amount of inorganic material. Bacterial community analysis using pyrosequencing analysis of 16S rRNA gene showed a predominance of members of the order Clostridiales, including members of genera Clostridium and Lutispora, which contain known cellulolytic organisms. Most differences among the samples were attributed to small taxonomic groups represented by  $\leq 10\%$  of total sequences.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Department of Animal Science, Ohio State University  
Contributors: Carver, S. M., Nelson, M. C., Yu, Z., Tuovinen, O. H.  
Number of pages: 12  
Pages: 11-22  
Publication date: 1 Apr 2015  
Peer-reviewed: Yes

#### Publication information

Journal: Biomass & Bioenergy

Volume: 75

ISSN (Print): 0961-9534

Ratings:

Scopus rating (2015): CiteScore 6.8 SJR 1.51 SNIP 1.587

Original language: English

ASJC Scopus subject areas: Agronomy and Crop Science, Forestry, Renewable Energy, Sustainability and the Environment, Waste Management and Disposal

Keywords: Anaerobic biodegradation, Biohydrogen, Cellulose biodegradation, Fermentation, Plant polymers

DOIs:

10.1016/j.biombioe.2015.02.005

URLs:

<http://www.scopus.com/inward/record.url?scp=84923621284&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84923621284

Research output: Contribution to journal > Article > Scientific > peer-review

#### From partial to complete optical erasure of azobenzene-polymer gratings: effect of molecular weight

##### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Frontier Photonics, Aalto University

Contributors: Vapaavuori, J., Ras, R. H. A., Kaivola, M., Bazuin, C. G., Priimägi, A.

Number of pages: 6

Pages: 11011-11016

Publication date: 2015

Peer-reviewed: Yes

##### Publication information

Journal: Journal of Materials Chemistry C

Volume: 3

Issue number: 42

ISSN (Print): 2050-7526

Ratings:

Scopus rating (2015): CiteScore 5.6 SJR 1.713 SNIP 1.488

Original language: English

DOIs:

10.1039/C5TC01776A

URLs:

<http://pubs.rsc.org/en/content/articlelanding/2015/tc/c5tc01776a#!divAbstract>

Research output: Contribution to journal > Article > Scientific > peer-review

#### High- and low-adhesive superhydrophobicity on the liquid flame spray-coated board and paper: structural effects on surface wetting and transition between the low- and high-adhesive states

##### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Energy and Process Engineering, Department of Physics, Engineering materials science and solutions (EMASS)

Contributors: Teisala, H., Tuominen, M., Aromaa, M., Stepien, M., Mäkelä, J. M., Saarinen, J. J., Toivakka, M., Kuusipalo, J.

Pages: 447-455

Publication date: 2013

Peer-reviewed: Yes

### Publication information

Journal: Colloid and Polymer Science

Volume: 291

Issue number: 2

ISSN (Print): 0303-402X

Ratings:

Scopus rating (2013): CiteScore 3.4 SJR 0.778 SNIP 0.943

Original language: English

DOIs:

10.1007/s00396-012-2833-5

### Bibliographical note

Jako 50% - 50% : : Poistettu tupla r=3313<br/>Contribution: organisation=epr,FACT1=0.5<br/>Contribution:

organisation=fys,FACT2=0.5<br/>Publisher name: Springer

Source: researchoutputwizard

Source ID: 3524

Research output: Contribution to journal > Article > Scientific > peer-review

### High temperature oxidation tests for the high velocity solution precursor flame sprayed manganese-cobalt oxide spinel protective coatings on SOFC interconnector steel

High velocity solution precursor flame spray process was used to deposit MnCo<sub>1.9</sub>Fe<sub>0.1</sub>O<sub>4</sub> and Mn<sub>1.5</sub>Co<sub>1.5</sub>O<sub>4</sub> coatings on Crofer 22 APU ferritic stainless steel samples. The solution precursors were manufactured by diluting metal nitrates into deionized water. The as-sprayed coatings were oxidized at 850 degrees C for 500 h to evaluate Cr-barrier and electrical properties.

The post-mortem studies were performed with various qualitative and quantitative elemental analysis methods and a four-point measurement was used for the area specific resistance studies. The as-sprayed coatings were formed of single crystallite nanoparticles (10-20 nm) and polycrystalline sub-micron particles (100-500 nm). The small particle and crystallite size showed strong sintering behavior during the oxidation cycle. Cr-migration was fully prevented through the oxidized coatings. The surface topography and grain growth dominated the electrical properties during the test cycle. Copyright (C) 2015, Hydrogen Energy Publications, LLC. Published by Elsevier Ltd. All rights reserved.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Surface Engineering, Research group: Materials Characterization, Research group: Ceramic materials, Engineering materials science and solutions (EMASS), Univ Toronto, University of Toronto, Dept Mat Sci & Engr, Univ Toronto, University of Toronto, Dept Mech & Ind Engr

Contributors: Puranen, J., Laakso, J., Honkanen, M., Heinonen, S., Kylvälähti, M., Lugowski, S., Coyle, T. W., Kesler, O., Vuoristo, P.

Number of pages: 12

Pages: 6216-6227

Publication date: 18 May 2015

Peer-reviewed: Yes

### Publication information

Journal: International Journal of Hydrogen Energy

Volume: 40

Issue number: 18

ISSN (Print): 0360-3199

Ratings:

Scopus rating (2015): CiteScore 6 SJR 1.27 SNIP 1.324

Original language: English

Keywords: High velocity solution precursor flame spray, SOFC interconnect, Protective coating, FUEL-CELLS, ELECTRICAL-CONDUCTIVITY, SOLID-SOLUTION, MN

DOIs:

10.1016/j.ijhydene.2015.02.129

Source: WOS

Source ID: 000354154300024

Research output: Contribution to journal > Article > Scientific > peer-review

### **High-temperature slurry erosion of vinylester matrix composites – The effect of test parameters**

Glass fibre (GF) reinforced vinylester composites (VE-FRP) are commonly used materials in hydrometallurgical reactors, the pulp and paper industry and waste water treatment plants, due to their excellent chemical resistance combined with good mechanical performance. In these applications, materials can be subjected to erosion, elevated temperatures (as high as 95 °C) and various chemical environments. However, studies on the slurry erosion of vinylester-based composites at high temperatures have not yet been reported. In this study, the erosion resistance of GF reinforced VE-FRP was investigated with a pilot-scale reactor. The effect of slurry concentration, erodent particle kinetic energy and slurry temperature was studied. The dominating wear mechanism was found to be abrasive wear. The VE-FRP structure was found to be prone to erosive turbulent flow and cavitation. Moreover, an increase in the erodent concentration of the slurry (10-20. wt%) or in the total kinetic energy of the erodent particles (30-770. kJ) increased the wear rate of the material markedly (up to 6 times higher weight loss). However, the total effect of different interrelated parameters was found to be complex. Consequently, it is recommended that predictions of the erosion rate of VE-FRP components are based on tests carried out in conditions that simulate the actual service environment.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Engineering materials science and solutions (EMASS), Outotec Research Center

Contributors: Sarlin, E. L., Lindgren, M., Suihkonen, R. J., Siljander, S. M. K., Kakkonen, M. M. S., Vuorinen, J. E.

Number of pages: 10

Pages: 488-497

Publication date: 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Wear

Volume: 328-329

ISSN (Print): 0043-1648

Ratings:

Scopus rating (2015): CiteScore 4.2 SJR 1.512 SNIP 2.027

Original language: English

Keywords: Vinylester, FRP, Glass fibre, Erosion, Slurry

Electronic versions:

Sarlin\_2015\_W. Embargo ended: 30/03/17

DOIs:

10.1016/j.wear.2015.03.021

URLs:

<http://urn.fi/URN:NBN:fi:tty-201606134243> . Embargo ended: 30/03/17

Research output: Contribution to journal > Article > Scientific > peer-review

### **Impact of mechanical and enzymatic pretreatments on softwood pulp fiber wall structure studied with NMR spectroscopy and X-ray scattering**

Dissolution of wood pulp can be enhanced by applying certain pretreatments before exposing the fibers to solvents. We have analyzed effect of mechanical and enzymatic pretreatments on softwood fiber wall structure using nuclear magnetic resonance (NMR) spectroscopic methods, small and wide angle X-ray scattering (SAXS, WAXS). NMR diffusometry was used to estimate the effect of pretreatments on average pore sizes at micrometer size scale and for the connectivity of the porous network. A proton NMR experiment was used to quantify the nonfreezing water content inside the fiber wall, and solid state NMR C-13 cross polarization (CP) magic angle spinning (MAS) spectroscopy was used to observe the effect of pretreatments on crystallinity and lateral fibril dimensions of cellulose fibrils, and in combination with fiber saturation point measurement to calculate the average pore size at nanometer size scale. Both WAXS and CP MAS NMR experiments confirmed that there were no changes in crystallinity nor in fibril lateral dimensions due to pretreatments. The pretreatments caused an increase in the amount of nonfreezing water, suggesting an opening of the pore system. According to diffusion experiments there are only minor changes in micrometer scale pore network due to pretreatments. SAXS results indicated that enzymatic treatment increased the microfibrillar distance, and there was also an increase in cross relaxation rate of magnetization from water to cellulose protons as observed by NMR. These were interpreted to be due to opening of microfibrillar bundles, leading to an increased accessibility of water.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Fibre Materials, Department of Materials Science, Univ Helsinki, University of Helsinki, Dept Phys, Aalto Univ, Aalto University, Sch Chem Technol, Dept Forest Prod Technol, VTT Tech Res Ctr Finland, VTT Technical Research Center Finland, Univ Helsinki, University of Helsinki, Polymer Chem Lab

Contributors: Virtanen, T., Penttilä, P. A., Maloney, T. C., Grönqvist, S., Kamppuri, T., Vehviläinen, M., Serimaa, R., Maunu, S. L.

Number of pages: 12  
Pages: 1565-1576  
Publication date: Jun 2015  
Peer-reviewed: Yes

#### Publication information

Journal: Cellulose  
Volume: 22  
Issue number: 3  
ISSN (Print): 0969-0239  
Ratings:

Scopus rating (2015): CiteScore 5.2 SJR 1.122 SNIP 1.202

Original language: English

Keywords: Softwood pulp, NMR spectroscopy, Diffusion, Enzymatic hydrolysis, SAXS, WAXS, CELLULOSE FIBRIL AGGREGATION, NUCLEAR-MAGNETIC-RESONANCE, SELF-DIFFUSION, DISSOLVING PULP, POROUS-MEDIA, WOOD FIBERS, FIELD GRADIENT, CHEMICAL PULP, IONIC LIQUIDS, KRAFT PULP

DOIs:

10.1007/s10570-015-0619-x

#### Bibliographical note

publication\_forum:53222

Source: WOS

Source ID: 000354193000009

Research output: Contribution to journal > Article > Scientific > peer-review

#### Improving Recovery Boiler Availability through Understanding Fume Behavior

Unexpected recovery boiler shutdowns are rare, but they can cost millions of dollars in lost income. Sometimes the inorganic compounds in black liquor can cause sudden fouling or plugging problems that could not be predicted beforehand. The ash particles can be divided into two main types and size classes: carryover and fume. This paper focuses on the smaller fume particles that form through the condensation of alkali metal vapors, and that deposit via different mechanisms than carryover. The location of fume deposition depends on several factors, such as flue gas and superheater temperatures, black liquor composition, and the flow field in the boiler.

This paper presents results obtained with a computational method that simulates fume formation in recovery boilers. The results in this paper focus on the effect of black liquor composition and elemental release on fume behavior, and the paper suggests how these observations should be taken into account when designing new boilers or retrofits. Moreover, the paper introduces the possible applications of the modeling method. These include, for example, troubleshooting of fouling problems in existing boilers, designing superheater configurations for new boilers, and positioning soot blowers.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Power Plant and Combustion Technology, Valmet Technologies Oy

Contributors: Leppänen, A., Välimäki, E.

Pages: 187-193

Publication date: Mar 2016

Peer-reviewed: Yes

#### Publication information

Journal: TAPPI Journal

Volume: 15

Issue number: 3

ISSN (Print): 0734-1415

Ratings:

Scopus rating (2016): SJR 0.377 SNIP 0.684

Original language: English

Research output: Contribution to journal > Article > Scientific > peer-review

#### Improving the extensibility, wet web and dry strength of paper by addition of agar

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science  
Contributors: Vishtal, A., Retulainen, E.  
Number of pages: 10  
Pages: 434-443  
Publication date: 2014  
Peer-reviewed: Yes

#### Publication information

Journal: Nordic Pulp and Paper Research Journal  
Volume: 29  
Issue number: 3  
ISSN (Print): 0283-2631  
Ratings:  
Scopus rating (2014): CiteScore 1.7 SJR 0.473 SNIP 0.868  
Original language: English

#### Bibliographical note

Contribution: organisation=mol,FACT1=1<br/>Portfolio EDEND: 2015-01-22  
Source: researchoutputwizard  
Source ID: 1759  
Research output: Contribution to journal > Article > Scientific > peer-review

#### Light-fuelled freestyle self-oscillators

Self-oscillation is a phenomenon where an object sustains periodic motion upon non-periodic stimulus. It occurs commonly in nature, a few examples being heartbeat, sea waves and fluttering of leaves. Stimuli-responsive materials allow creating synthetic self-oscillators fuelled by different forms of energy, e.g. heat, light and chemicals, showing great potential for applications in power generation, autonomous mass transport, and self-propelled micro-robotics. However, most of the self-oscillators are based on bending deformation, thereby limiting their possibilities of being implemented in practical applications. Here, we report light-fuelled self-oscillators based on liquid crystal network actuators that can exhibit three basic oscillation modes: bending, twisting and contraction-expansion. We show that a time delay in material response dictates the self-oscillation dynamics, and realize a freestyle self-oscillator that combines numerous oscillation modes simultaneously by adjusting the excitation beam position. The results provide new insights into understanding of self-oscillation phenomenon and offer new designs for future self-propelling micro-robots.

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Materials Science and Environmental Engineering, Research group: Chemistry & Advanced Materials  
Contributors: Zeng, H., Lahikainen, M., Liu, L., Ahmed, Z., Wani, O. M., Wang, M., Yang, H., Priimagi, A.  
Publication date: 7 Nov 2019  
Peer-reviewed: Yes

#### Publication information

Journal: Nature Communications  
Volume: 10  
Issue number: 1  
Article number: 5057  
ISSN (Print): 2041-1723  
Ratings:  
Scopus rating (2019): CiteScore 18.1 SJR 5.569 SNIP 2.847  
Original language: English  
Electronic versions:  
Light-fuelled freestyle self-oscillators 2019  
DOIs:  
10.1038/s41467-019-13077-6  
URLs:  
<http://urn.fi/URN:NBN:fi:tuni-202003032499>  
Source: PubMed  
Source ID: 31700006  
Research output: Contribution to journal > Article > Scientific > peer-review

#### Low temperature temporal and spatial atomic layer deposition of TiO<sub>2</sub> films

Titanium dioxide films were grown by atomic layer deposition (ALD) using titanium tetraisopropoxide as a titanium precursor and water, ozone, or oxygen plasma as coreactants. Low temperatures (80-120 degrees C) were used to grow moisture barrier TiO<sub>2</sub> films on polyethylene naphthalate. The maximum growth per cycle for water, ozone, and oxygen

plasma processes were 0.33, 0.12, and 0.56 angstrom/cycle, respectively. X-ray photoelectron spectrometry was used to evaluate the chemical composition of the layers and the origin of the carbon contamination was studied by deconvoluting carbon C1s peaks. In plasma-assisted ALD, the film properties were dependent on the energy dose supplied by the plasma. TiO<sub>2</sub> films were also successfully deposited by using a spatial ALD (SALD) system based on the results from the temporal ALD. Similar properties were measured compared to the temporal ALD deposited TiO<sub>2</sub>, but the deposition time could be reduced using SALD. The TiO<sub>2</sub> films deposited by plasma-assisted ALD showed better moisture barrier properties than the layers deposited by thermal processes. Water vapor transmission rate values lower than  $5 \times 10^{-4}$  g day<sup>-1</sup> m<sup>-2</sup> (38 degrees C and 90% RH) was measured for 20 nm of TiO<sub>2</sub> film deposited by plasma-assisted ALD. (C) 2015 American Vacuum Society.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Lappeenranta Univ Technol, Lappeenranta University of Technology, Lab Green Chem, ASTRaL Grp, Eindhoven Univ Technol, Eindhoven University of Technology, Dept Appl Phys, Masaryk Univ, Masaryk University Brno, R&D Ctr Low Cost Plasma & Nanotechnol Surface Mod

Contributors: Aghaee, M., Maydannik, P. S., Johansson, P., Kuusipalo, J., Creatore, M., Homola, T., Cameron, D. C.

Number of pages: 9

Publication date: Jul 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Vacuum Science & Technology A

Volume: 33

Issue number: 4

Article number: 041512

ISSN (Print): 1553-1813

Original language: English

Keywords: DIOXIDE THIN-FILMS, BINARY REACTION SEQUENCE, TITANIUM-DIOXIDE, BARRIER PROPERTIES, ROOM-TEMPERATURE, PLASMA, AL<sub>2</sub>O<sub>3</sub>, ISOPROPOXIDE, PASSIVATION, PRECURSOR

DOIs:

10.1116/1.4922588

Source: WOS

Source ID: 000357826400024

Research output: Contribution to journal > Article > Scientific > peer-review

#### Machine-coated starch-based dispersion coatings prevent mineral oil migration from paperboard

Mineral oil migration through paperboard presents a safety risk in modern food packaging. This study aimed to enhance the safety of fiber-based packaging by utilizing a bio-based composite barrier layer to protect against mineral oil. Starch-clay composite coatings on paperboard were created via dispersion coating. Thermal analysis of the coating components and field emission scanning electron microscopy imaging were performed to ascertain the physicochemical properties and morphology of the coatings. Coating functionality was evaluated using contact angles and transmission rate (water and oxygen) measurements. The packaging safety focus was implemented by measuring the gas phase migration of heptane and analyzing the migration of liquid mineral oil through the coated paperboards with FTIR. The functional properties of the coated paperboards were maintained or improved. The studied coatings were effective barriers against the migration of mineral oil and could hence improve the barrier properties and safety of fiber-based primary food packaging.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Paper Converting and Packaging

Contributors: Koivula, H. M., Jalkanen, L., Saukkonen, E., Ovaska, S., Lahti, J., Christophliemk, H., Mikkonen, K. S.

Pages: 173-181

Publication date: 2016

Peer-reviewed: Yes

#### Publication information

Journal: Progress in Organic Coatings

Volume: 99

ISSN (Print): 0300-9440

Ratings:

Scopus rating (2016): CiteScore 4.6 SJR 0.852 SNIP 1.36

Original language: English

Keywords: Mineral oil migration; Barrier; Dispersion coating; Paperboard; Food packaging

DOIs:

10.1016/j.porgcoat.2016.05.017

Research output: Contribution to journal › Article › Scientific › peer-review

### Measuring synthesis yield in graphene oxide synthesis by modified hummers method

Synthesis of graphene oxide by the modified Hummers method and measuring the synthesis yield were investigated. Based on the results, a comprehensive method to measure graphene oxide synthesis yield was proposed, which will allow comparison of future literature results. In addition, changes are proposed to the exfoliation procedure to improve the yield of the modified Hummers synthesis. With the proposed method, systematic error of the concentration measurement was calculated to be  $\pm 0.08 \times 10^{-3}$  g mL<sup>-1</sup>. In addition, changes proposed to the graphene oxide exfoliation process can improve the synthesis yield by up to 70%.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Ceramic materials, Tampere University of Technology, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Materials Characterization, Engineering materials science and solutions (EMASS), University of Helsinki

Contributors: Frankberg, E. J., George, L., Efimov, A., Honkanen, M., Pessi, J., Levänen, E.

Number of pages: 5

Pages: 755-759

Publication date: 2 Sep 2015

Peer-reviewed: Yes

#### Publication information

Journal: Fullerenes Nanotubes and Carbon Nanostructures

Volume: 23

Issue number: 9

ISSN (Print): 1536-383X

Ratings:

Scopus rating (2015): CiteScore 1.9 SJR 0.278 SNIP 0.605

Original language: English

ASJC Scopus subject areas: Organic Chemistry, Physical and Theoretical Chemistry, Materials Science(all), Atomic and Molecular Physics, and Optics

Keywords: Concentration, Graphene oxide, Hummers method, Synthesis, Yield

Electronic versions:

Frankberg\_revised\_text\_print

DOIs:

10.1080/1536383X.2014.993754

URLs:

<http://urn.fi/URN:NBN:fi:tty-201603173654>

#### Bibliographical note

Versio ja lupa ok 26.1.2016 KK

Source: Scopus

Source ID: 84929598253

Research output: Contribution to journal › Article › Scientific › peer-review

### Methane thermal decomposition in regenerative heat exchanger reactor: Experimental and modeling study

In this work, thermal decomposition of methane (TDM) was experimentally studied at nominal gas temperatures of 1070 K–1450 K in a non-catalytic laboratory test reactor. The purpose was to use a simple kinetic mechanism to describe the TDM reaction, which could be applied in industrial reactor design. The experimental data was utilized to optimize global kinetic parameters describing the TDM reaction in the test reactor. For comparison, a 37-step reaction mechanism for TDM was adopted from the literature. When analyzing experimental datasets from the literature, the optimized global kinetics provided better agreement with the experimental data than the 37-step mechanism when the reactor temperature profiles were defined in detail. Since the 37-step mechanism was not able to predict the solid carbon formation well enough, the mechanism was slightly adjusted according to a reaction flow and sensitivity analysis. Additionally, it was suggested that the 37-step mechanism can be improved by optimizing the reaction mechanism by using a detailed experimental data of hydrocarbon formation in TDM achieved in an environment where the temperature profiles are fully defined.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Chemistry and Bioengineering, Research group: Bio- and Circular Economy, Norwegian University of Science and Technology, NTNU



Contributors: Keipi, T., Li, T., Løvås, T., Tolvanen, H., Konttinen, J.  
Pages: 823-832  
Publication date: 15 Sep 2017  
Peer-reviewed: Yes

#### Publication information

Journal: Energy  
Volume: 135  
ISSN (Print): 0360-5442  
Ratings:

Scopus rating (2017): CiteScore 8.1 SJR 1.99 SNIP 1.946

Original language: English

Keywords: CCS, Hydrogen production, Kinetics, Methane cracking, Methane decomposition

DOIs:

10.1016/j.energy.2017.06.176

Research output: Contribution to journal > Article > Scientific > peer-review

#### Microstructure-property relationships of novel ultra-high strength press hardening steels

The industrial significance of microalloyed martensitic steels manufactured via cold rolling, re-austenitization, and quenching has been typically recognized as low. However, it is currently believed that microalloying can improve the in-service properties of ultra-high-strength press hardening steels. In this work, five 34MnB5-based steels were designed to address the role of Ti and V when combined with Cr or Mo. Microstructure-property relationships were analyzed after die quenching and additional bake hardening (BH) heat treatment using advanced methods of microscopy, glow discharge optical emission spectroscopy, quasi-static tensile tests, and three-point bending tests. Results indicate that both Ti and V can provide grain size refinement through the formation of stable nanosized precipitates. The BH treatment improved postuniform elongation values, indicating a trend of improved ductility. However, the expected improvements in bendability were clearly confirmed only for two V-microalloyed steels with the alloying concepts of 0.3Cr-0.15V-0.03Al-0.02Ti-0.0020B and 0.3Mo-0.15V-0.0060N (without Al-Ti-B additions) (wt pct). Thus, it was discovered that microalloying with V, when combined with either Cr or Mo, provides a promising combination of mechanical properties as far as the austenitization parameters are appropriately controlled.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Research group: Metals Technology, Research group: Materials Characterization, SSAB Europe Oy

Contributors: Järvinen, H., Honkanen, M., Oja, O., Järvenpää, M., Peura, P.

Number of pages: 21

Pages: 816-836

Publication date: 2019

Peer-reviewed: Yes

Early online date: 29 Nov 2018

#### Publication information

Journal: Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science

Volume: 50

Issue number: 2

ISSN (Print): 1073-5623

Ratings:

Scopus rating (2019): CiteScore 3.9 SJR 0.906 SNIP 1.22

Original language: English

ASJC Scopus subject areas: Condensed Matter Physics, Mechanics of Materials, Metals and Alloys

Keywords: Press hardening, Bake hardening, Martensite, EBSD, TEM, Mechanical behavior

Electronic versions:

Microstructure-property\_relationships\_2018. Embargo ended: 29/11/19

DOIs:

10.1007/s11661-018-4967-7

URLs:

<http://urn.fi/URN:NBN:fi:tuni-201912307139>. Embargo ended: 29/11/19

Research output: Contribution to journal > Article > Scientific > peer-review

#### Modelling fume deposit growth in recovery boilers: effect of flue gas and deposit temperature

The high ash content of black liquor causes fouling problems in the Kraft recovery boiler. The ash-forming elements condense into submicron-sized fume particles in the superheater area and the boiler bank and can deposit on heat-

transfer surfaces. The fume deposits can then lower heat-transfer rate, plug flue gas flow, and expose surfaces to corrosion. This paper presents the results of a sensitivity analysis obtained using a CFD (computational fluid dynamics)-based sub-model of the formation of fume particles and deposits, showing how flue gas and deposit surface temperatures affect instantaneous fume deposit growth. The results indicate that fume deposit growth is a self-limiting process because the growth rate decreases as the deposit surface temperature increases. On the other hand, increasing the flue gas temperature increases the fume deposition rate when the element release factors are kept constant.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Power Plant and Combustion Technology, University of Toronto, Canada, Valmet Technologies Oy

Contributors: Leppänen, A., Tran, H., Välimäki, E., Oksanen, A.

Number of pages: 8

Pages: 50-57

Publication date: 2014

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Science and Technology for Forest Products and Processes

Volume: 4

Issue number: 1

ISSN (Print): 1927-6311

Ratings:

Scopus rating (2014): SJR 0.239 SNIP 0.28

Original language: English

URLs:

<http://www.paptac.ca/en/publications/jfor>

#### Bibliographical note

Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2014-12-12<br/>Publisher name: PAPTAC, Pulp and Paper Technical Association of Canada

Source: researchoutputwizard

Source ID: 924

Research output: Contribution to journal > Article > Scientific > peer-review

#### N-Alkyl ammonium resorcinarene salts: multivalent halogen-bonded deep-cavity cavitands

N-Cyclohexyl ammonium resorcinarene halides, stabilized by an intricate array of hydrogen bonds in a cavitand-like assembly, form multivalent halogen-bonded deep-cavity cavitands with perfluoriodobenzenes. As observed from the macromolar to infinite concentration range through crystal growth and single crystal X-ray analyses, four 1,4-diiodotetrafluorobenzenes form moderate halogen bonds with the bromides of the N-cyclohexyl ammonium resorcinarene bromides leading to a deep-cavity cavitand-like structure. In this assembly, the N-cyclohexyl ammonium resorcinarene bromide also acts as a guest and sits in the upper cavity of the assembly interacting with the 1,4-diiodotetrafluorobenzene through strong pi center dot center dot pi interactions. Solvent molecules act as guests and are located deep in the cavity of the resorcinarene skeleton. In the millimolar range, H-1 and F-19 NMR spectroscopic analyses confirm halogen bonding in solution. Fast exchange binding of electron rich fluorophores (naphthalene, anthracene and pyrene) in the upper layer of these assemblies was also observed in the millimolar range while in the micromolar range, using fluorescence analysis, no binding of the fluorophores was observed.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Univ Jyväskylä, University of Jyväskylä, Dept Chem, Nanosci Ctr

Contributors: Beyeh, N. K., Valkonen, A., Bhowmik, S., Pan, F., Rissanen, K.

Number of pages: 6

Pages: 340-345

Publication date: 2015

Peer-reviewed: Yes

#### Publication information

Journal: Organic chemistry frontiers

Volume: 2

Issue number: 4

ISSN (Print): 2052-4129

Ratings:

Scopus rating (2015): CiteScore 3.4 SJR 2.31 SNIP 0.877

Original language: English

Keywords: ELECTRON DONOR SOLVENTS, RECOGNITION, ANALOGS, SHIFTS

DOIs:

10.1039/c4qo00326h

Source: WOS

Source ID: 000364444500006

Research output: Contribution to journal > Article > Scientific > peer-review

## Nanoparticle Deposition from Liquid Flame Spray onto Moving Roll-to-Roll Paperboard Material

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Physics, Department of Energy and Process Engineering, Engineering materials science and solutions (EMASS)

Contributors: Mäkelä, J. M., Aromaa, M., Teisala, H., Tuominen, M., Stepien, M., Saarinen, J. J., Toivakka, M., Kuusipalo, J.

Pages: 827-837

Publication date: 2011

Peer-reviewed: Yes

### Publication information

Journal: Aerosol Science and Technology

Volume: 45

Issue number: 7

ISSN (Print): 0278-6826

Ratings:

Scopus rating (2011): CiteScore 4.2 SJR 1.312 SNIP 1.043

Original language: English

DOIs:

10.1080/02786826.2011.566292

### Bibliographical note

Contribution: organisation=fys,FACT1=0.5<br/>Contribution: organisation=epr pap,FACT2=0.5

Source: researchoutputwizard

Source ID: 6697

Research output: Contribution to journal > Article > Scientific > peer-review

## Nanostructures Increase Water Droplet Adhesion on Hierarchically Rough Superhydrophobic Surfaces

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research area: Aerosol Physics, Department of Energy and Process Engineering, Department of Physics, Engineering materials science and solutions (EMASS)

Contributors: Teisala, H., Tuominen, M., Aromaa, M., Stepien, M., Mäkelä, J. M., Saarinen, J. J., Toivakka, M., Kuusipalo, J.

Pages: 3138-3145

Publication date: 2012

Peer-reviewed: Yes

### Publication information

Journal: Langmuir

Volume: 28

Issue number: 6

ISSN (Print): 0743-7463

Ratings:

Scopus rating (2012): CiteScore 7.4 SJR 2.179 SNIP 1.356

Original language: English

DOIs:

10.1021/la203155d

### Bibliographical note

Contribution: organisation=epr,FACT1=0.5<br/>Contribution: organisation=fys,FACT2=0.5<br/>Publisher name: American Chemical Society

Source: researchoutputwizard

Source ID: 5410

Research output: Contribution to journal > Article > Scientific > peer-review

### Noncovalent functionalization of reduced graphene oxide with pluronic F127 and its nanocomposites with gum arabic

Nanocomposites of pluronic F127 modified reduced graphene oxide (PF127-rGO) with polyethylene glycol plasticize gum arabic (PGA) was prepared by evaporating an aqueous solution mixture of PF127-rGO and PGA. PF127-rGO was synthesized by the in-situ reduction of graphene oxide using hydrazine in presence of pluronic F127 and characterized by the Uv-Vis spectroscopy, transmission electron microscopy (TEM), wide angle x-ray scattering (WAXS), Fourier transforms infrared spectroscopy (FTIR), thermogravimetric analysis (TGA) and Raman spectroscopy. The Uv-Vis and Raman spectroscopy results indicate that pluronic F127 functionalization does not hamper the structure of rGO, and TEM image indicates, the pluronic F127 anchored rGO sheets remain exfoliated in diluted aqueous solution of PF127-rGO. WAXS, FTIR and TGA studies confirms the functionalization of rGO with pluronic F127. PF127-rGO 2.5, PF127-rGO 5 and PF127-rGO 7.5 nanocomposites were fabricated, where the numbers represent the weight percentage of PF127-rGO with respect to PGA. The composite films were characterized by field emission scanning electron microscopy (FESEM), FTIR, WAXS and mechanical property study. FESEM and WAXS studies show good dispersion of PF127-rGO sheets in the PGA matrix. The FTIR results indicate a significant interaction between functional groups of PF127-rGO and functional groups of PGA. PF127-rGO 7.5 shows a 124% increase of stress at break and 185% increase of Young's modulus compared to pure PGA.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Research group: Plastics and Elastomer Technology, Khulna University of Engineering & Technology (KUET), Chonbuk National University, Swinburne University of Technology

Contributors: Layek, R. K., Uddin, M. E., Kim, N. H., Tak Lau, A. K., Lee, J. H.

Number of pages: 9

Pages: 155-163

Publication date: 1 Nov 2017

Peer-reviewed: Yes

### Publication information

Journal: Composites Part B : Engineering

Volume: 128

ISSN (Print): 1359-8368

Ratings:

Scopus rating (2017): CiteScore 9.3 SJR 2.039 SNIP 2.106

Original language: English

ASJC Scopus subject areas: Ceramics and Composites, Mechanics of Materials, Mechanical Engineering, Industrial and Manufacturing Engineering

Keywords: Electron microscopy, Mechanical properties, Nano-structures, Polymer-matrix composites (PMCs), Thermal analysis

DOIs:

10.1016/j.compositesb.2017.07.010

Source: Scopus

Source ID: 85024888498

Research output: Contribution to journal > Article > Scientific > peer-review

### Numerical modeling of fine particle and deposit formation in a recovery boiler

In kraft pulp mills, black liquor is concentrated and burned in recovery boilers to produce steam and power and to recover pulping chemicals. Black liquor contains a large amount of alkali compounds, which form ash with low melting temperatures upon combustion. This causes many problems in recovery boiler operation, including fouling of the heat transfer surfaces, plugging of the flue gas passages, reduction of the heat transfer rate, and corrosion of the superheater tubes. This paper presents a model for simulating fine fume particles formed as a result of condensation of alkali compound vapors in the recovery boiler. The modeling method combines CFD modeling, equilibrium chemistry, and fine particle dynamics in a way that enables simulation of a full scale three-dimensional boiler environment. The model has been partially validated with measurements performed in an operating recovery boiler. The modeling results, particularly for the fume particle composition, agree well with the actual measurements. (C) 2014 Elsevier Ltd. All rights reserved.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Power Plant and Combustion Technology, Urban circular bioeconomy (UrCirBio), University of Toronto, Canada, VTT Technical Research Centre of Finland, Valmet Technologies Oy

Contributors: Leppänen, A., Tran, H., Taipale, R., Välimäki, E., Oksanen, A.

Number of pages: 9

Pages: 45-53

Publication date: 1 Aug 2014

Peer-reviewed: Yes

Early online date: 16 Apr 2014

### Publication information

Journal: Fuel

Volume: 129

ISSN (Print): 0016-2361

Ratings:

Scopus rating (2014): CiteScore 5.6 SJR 1.634 SNIP 2.29

Original language: English

Keywords: Kraft recovery boiler, Alkali metal, Fine particle, Deposition, Computational fluid dynamics, FUME FORMATION, BLACK LIQUOR, COMBUSTION, BEHAVIOR, DUST

Electronic versions:

leppanen\_numerical\_modeling\_of\_fine\_particle

DOIs:

10.1016/j.fuel.2014.03.046

URLs:

<http://urn.fi/URN:NBN:fi:tty-201412051586>

### Bibliographical note

Contribution: organisation=keb,FACT1=1<br/>Portfolio EDEND: 2014-04-29<br/>Publisher name: Elsevier Ltd

Source: researchoutputwizard

Source ID: 922

Research output: Contribution to journal > Article > Scientific > peer-review

### On the effect of deformation twinning and microstructure to strain hardening of high manganese austenitic steel 3D microstructure aggregates at large strains

The hardening and deformation characteristics of Hadfield microstructure are studied to investigate the effect of microstructure to the material behavior. A crystal plasticity model including dislocation slip and deformation twinning is employed. The role of deformation twinning to the overall strain hardening of the material is evaluated for two different grain structures. Large compressive strains are applied on 3D microstructural aggregates representing the uniform and non-uniform grain structures of Hadfield steels. The grain structure has an effect on the strain hardening rate as well as on the overall hardening capability of the microstructure. A major reason causing the difference in strain hardening arises from the different twin volume fraction evolution influenced by intra-grain and inter-grain interactions. A mixture of large and small grains was found to be more favorable for twinning and thus resulting in a greater hardening capability than uniform grain size.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Research group: Materials Characterization, VTT Lifecycle Solutions

Contributors: Lindroos, M., Laukkanen, A., Cailletaud, G., Kuokkala, V.

Pages: 68-76

Publication date: 2017

Peer-reviewed: Yes

### Publication information

Journal: International Journal of Solids and Structures

Volume: 125

ISSN (Print): 0020-7683

Ratings:

Scopus rating (2017): CiteScore 4.8 SJR 1.295 SNIP 1.574

Original language: English

ASJC Scopus subject areas: Modelling and Simulation, Materials Science(all), Condensed Matter Physics, Mechanics of Materials, Mechanical Engineering, Applied Mathematics

Keywords: Austenitic manganese steel, Crystal plasticity, Deformation twinning, Microstructure based modeling

DOIs:

10.1016/j.ijsostr.2017.07.015

#### Bibliographical note

EXT="Lindroos, Matti"

Source: Scopus

Source ID: 85025152227

Research output: Contribution to journal › Article › Scientific › peer-review

#### Perfluoro-1,1'-biphenyl and perfluoronaphthalene and their derivatives as $\pi$ -acceptors for anions

Addition of anions to perfluorinated 1,1'-biphenyl 1 or naphthalene 2 results in a shift of the  $^{19}\text{F}$  NMR signals. However, any specific interaction cannot be assigned to this effect. In order to study the interaction in more detail, the salt derivatives 3 and 4 were prepared and studied by single crystal X-ray diffraction revealing weak anion- $\pi$  interactions in the solid state.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, University of Jyväskylä, Institut für Organische Chemie, RWTH Aachen

Contributors: Yi, H., Albrecht, M., Valkonen, A., Rissanen, K.

Number of pages: 4

Pages: 746-749

Publication date: 1 Jan 2015

Peer-reviewed: Yes

#### Publication information

Journal: New Journal of Chemistry

Volume: 39

Issue number: 1

ISSN (Print): 1144-0546

Ratings:

Scopus rating (2015): CiteScore 4 SJR 0.935 SNIP 0.825

Original language: English

ASJC Scopus subject areas: Chemistry(all), Catalysis, Materials Chemistry

DOIs:

10.1039/c4nj01654h

URLs:

<http://www.scopus.com/inward/record.url?scp=84919782132&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84919782132

Research output: Contribution to journal › Article › Scientific › peer-review

#### Photocatalytic and antibacterial properties of ZnO films with different surface topographies on stainless steel substrate

Zinc oxide films with three types of topographies: needle-like and hexagonal rods and flakes, were prepared by hydrothermal synthesis on stainless steel substrates to investigate their photocatalytic and antibacterial properties. The photocatalytic activity was measured with a methylene blue (MB) discoloration test, whereas a method using bioluminescent whole cell bacterial biosensors enabling the constant monitoring of the amount of living cells on the surfaces was used here to study the antibacterial properties. The results showed that photocatalytic activity was clearly influenced by the surface area, which is in turn dependent on the topography. Moreover, it was found that all the examined films decreased notably the amount of *Staphylococcus aureus* and *Escherichia coli* on the surfaces. Despite significant differences in the surface areas of the studied samples that led to different zinc dissolution rate in aqueous environment, no notable differences in antibacterial activity between the films with different morphologies could be detected. These results are presented and discussed in this paper.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Ceramic materials, Department of Chemistry and Bioengineering, Research group: Industrial Bioengineering and Applied Organic Chemistry, VTT Technical Research Centre of Finland

Contributors: Heinonen, S., Kannisto, M., Nikkanen, J., Huttunen-Saarivirta, E., Karp, M., Levänen, E.

Number of pages: 8

Pages: 842-849

Publication date: 1 Oct 2016

Peer-reviewed: Yes

#### Publication information

Journal: Thin Solid Films

Volume: 616

ISSN (Print): 0040-6090

Ratings:

Scopus rating (2016): CiteScore 3.7 SJR 0.639 SNIP 0.863

Original language: English

ASJC Scopus subject areas: Electronic, Optical and Magnetic Materials, Surfaces and Interfaces, Surfaces, Coatings and Films, Metals and Alloys, Materials Chemistry

Keywords: Antibacterial, Biosensor cell, Hydrothermal synthesis, Photocatalytic activity, Zinc oxide

DOIs:

10.1016/j.tsf.2016.10.002

URLs:

<http://www.scopus.com/inward/record.url?scp=84991648557&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84991648557

Research output: Contribution to journal > Article > Scientific > peer-review

#### Pinacol-Derived Chlorohydrosilane in Metal-Free Reductive Amination for the Preparation of Tertiary Alkylphenolmethyl Amines

A new metal-free reductive amination protocol using a pinacol-derived chlorohydrosilane/pyridine system for the preparation of aminoalkylphenols is described. This method is selective toward iminiums derived from alkylphenol ketones under an in situ formation of a trialkoxyhydrosilane and activation with a Lewis base, as further indicated by computational studies. This method demonstrated high functional group tolerance affording an array of novel aminoalkylphenols in moderate to high yields with equimolar amounts of reactants and a wide substrate scope.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science and Environmental Engineering, Research group: Chemistry & Advanced Materials, Inst Super Tecn, Instituto Superior Tecnico, Universidade de Lisboa, CQE

Contributors: Assoah, B., Veiros, L. F., R. Candeias, N.

Number of pages: 5

Pages: 1402-1406

Publication date: 15 Feb 2019

Peer-reviewed: Yes

#### Publication information

Journal: Organic Letters

Volume: 21

Issue number: 5

ISSN (Print): 1523-7060

Ratings:

Scopus rating (2019): CiteScore 10.4 SJR 2.032 SNIP 1.194

Original language: English

Electronic versions:

[acs.orglett.9b00121](https://doi.org/10.1021/acs.orglett.9b00121)

DOIs:

10.1021/acs.orglett.9b00121

URLs:

<http://urn.fi/URN:NBN:fi:tty-201906281915>

Research output: Contribution to journal > Article > Scientific > peer-review

#### Preferential Attachments of Organic Dyes onto {101} Facets of TiO<sub>2</sub> Nanoparticles

Hybrid nanostructures of organic dyes/TiO<sub>2</sub> nanoparticles were successfully fabricated by self-assembly method: Compared with pure organic dyes, these hybrid nanostructures showed enhanced performance of light absorption. Extensive high-resolution transmission electron Microscopy observations demonstrated that the organic dyes are preferentially attached onto the {101} facets of anatase TiO<sub>2</sub> nanoparticles. Density functional theory calculations further confirmed that the preferential attachments are reasonable. These discoveries are very important

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research group: Supramolecular photochemistry, Department of Chemistry and Bioengineering, Frontier Photonics, Qingdao Univ, Qingdao University, Cultivat Base State Key Lab, Qingdao Univ, Qingdao University, Coll Chem Sci & Engrn, Qingdao Univ, Qingdao University, Coll Phys, Qingdao Univ, Qingdao University, Shandong University, Shandong Univ, Key Lab Photon Mat & Technol

Contributors: Diao, F., Liang, W., Tian, F., Wang, Y., Vivo, P., Efimov, A., Lemmetyinen, H.

Number of pages: 6

Pages: 8960-8965

Publication date: 23 Apr 2015

Peer-reviewed: Yes

#### Publication information

Journal: Journal of Physical Chemistry C

Volume: 119

Issue number: 16

ISSN (Print): 1932-7447

Ratings:

Scopus rating (2015): CiteScore 7.9 SJR 1.886 SNIP 1.246

Original language: English

Keywords: SENSITIZED SOLAR-CELLS, ANATASE, SURFACES, ADSORPTION, WATER, OXIDE

DOIs:

10.1021/acs.jpcc.5b01369

URLs:

<http://www.scopus.com/inward/record.url?scp=84928527015&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: WOS

Source ID: 000353603500062

Research output: Contribution to journal > Article > Scientific > peer-review

#### Remarkable Dependence of the Final Charge Separation Efficiency on the Donor-Acceptor Interaction in Photoinduced Electron Transfer

The unprecedented dependence of final charge separation efficiency as a function of donor-acceptor interaction in covalently-linked molecules with a rectilinear rigid oligo-p-xylene bridge has been observed. Optimization of the donor-acceptor electronic coupling remarkably inhibits the undesirable rapid decay of the singlet charge-separated state to the ground state, yielding the final long-lived, triplet charge-separated state with circa 100% efficiency. This finding is extremely useful for the rational design of artificial photosynthesis and organic photovoltaic cells toward efficient solar energy conversion.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Kyoto Women's University, Tokushima University, Kobe University, Japan Science and Technology Agency, University of Tokyo

Contributors: Higashino, T., Yamada, T., Yamamoto, M., Furube, A., Tkachenko, N. V., Miura, T., Kobori, Y., Jono, R., Yamashita, K., Imahori, H.

Pages: 629-633

Publication date: 2016

Peer-reviewed: Yes

#### Publication information

Journal: Angewandte Chemie (International Edition)

Volume: 55

Issue number: 2

ISSN (Print): 1433-7851

Ratings:

Scopus rating (2016): CiteScore 18.7 SJR 5.954 SNIP 2.185

Original language: English

ASJC Scopus subject areas: Chemistry(all), Catalysis

Keywords: Charge separation, Electron transfer, Electronic coupling, Exciplexes, Marcus theory

DOIs:

10.1002/anie.201509067

Source: Scopus

Source ID: 84958749577

Research output: Contribution to journal > Article > Scientific > peer-review



## **Silver-Decorated TiO<sub>2</sub> Inverse Opal Structure for Visible Light-Induced Photocatalytic Degradation of Organic Pollutants and Hydrogen Evolution**

TiO<sub>2</sub> inverse opal (TIO) structures were prepared by the conventional wet chemical method, resulting in well-formed structures for photocatalytic activity. The obtained structures were functionalized with liquid flame spray-deposited silver nanoparticles (AgNPs). The nanocomposites of TIO and AgNPs were extensively characterized by various spectroscopies such as UV, Raman, X-ray diffraction, energy-dispersive spectroscopy, and X-ray photoelectron spectroscopy combined with microscopic methods such as scanning electron microscopy, transmission electron microscopy (TEM), and high-resolution TEM. The characterization confirmed that high-quality heterostructures had been fabricated with evenly and uniformly distributed AgNPs. Fabrication of anatase TiO<sub>2</sub> was confirmed, and formation of AgNPs was verified with surface plasmon resonant properties. The photocatalytic activity results measured in the gas phase showed that deposition of AgNPs increases photocatalytic activity both under UVA and visible light excitation; moreover, enhanced hydrogen evolution was demonstrated under visible light.

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Physics, Research group: Aerosol Synthesis, Ita-Suomen yliopisto, St. Petersburg State University, Imperial College, London, 24.8.2012

Contributors: Temerov, F., Pham, K., Juuti, P., Mäkelä, J. M., Grachova, E. V., Kumar, S., Eslava, S., Saarinen, J. J.

Number of pages: 11

Pages: 41200-41210

Publication date: 16 Sep 2020

Peer-reviewed: Yes

### **Publication information**

Journal: ACS Applied Materials & Interfaces

Volume: 12

Issue number: 37

ISSN (Print): 1944-8244

Original language: English

ASJC Scopus subject areas: Materials Science(all)

Keywords: hydrogen evolution, liquid flame spray, photocatalysis, silver nanoparticles, TiO<sub>2</sub> inverse opal

DOIs:

10.1021/acsami.0c08624

### **Bibliographical note**

EXT="Saarinen, Jarkko J."

Source: Scopus

Source ID: 85091192016

Research output: [Contribution to journal](#) > [Article](#) > [Scientific](#) > [peer-review](#)

## **Surface chemical analysis of photocatalytic wettability conversion of TiO<sub>2</sub> nanoparticle coating**

### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Research area: Aerosol Physics, Department of Energy and Process Engineering, Department of Physics, Engineering materials science and solutions (EMASS)

Contributors: Stepien, M., Saarinen, J. J., Teisala, H., Tuominen, M., Aromaa, M., Kuusipalo, J., Mäkelä, J. M., Toivakka, M.

Pages: 73-79

Publication date: 2012

Peer-reviewed: Yes

### **Publication information**

Journal: Surface and Coatings Technology

Volume: 208

ISSN (Print): 0257-8972

Ratings:

Scopus rating (2012): CiteScore 3.6 SJR 1.041 SNIP 1.631

Original language: English

DOIs:

10.1016/j.surfcoat.2012.08.008

### Bibliographical note

Poistettu tupla r=2012.<br/>Contribution: organisation=epr,FACT1=0.5<br/>Contribution: organisation=fys,FACT2=0.5<br/>Publisher name: Elsevier  
Source: researchoutputwizard  
Source ID: 5351  
Research output: Contribution to journal > Article > Scientific > peer-review

### Surface chemical characterization of nanoparticle coated paperboard

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Research area: Aerosol Physics, Department of Energy and Process Engineering, Department of Physics, Engineering materials science and solutions (EMASS)  
Contributors: Stepien, M., Saarinen, J. J., Teisala, H., Tuominen, M., Aromaa, M., Kuusipalo, J., Mäkelä, J. M., Toivakka, M.  
Pages: 3119-3125  
Publication date: 2012  
Peer-reviewed: Yes

#### Publication information

Journal: Applied Surface Science  
Volume: 258  
Issue number: 7  
ISSN (Print): 0169-4332  
Ratings:  
Scopus rating (2012): CiteScore 3.5 SJR 0.913 SNIP 1.347  
Original language: English  
DOIs:  
10.1016/j.apsusc.2011.11.048

### Bibliographical note

Poistettu tupla r=773, 1835<br/>Contribution: organisation=epr pap,FACT1=0.5<br/>Contribution: organisation=fys,FACT2=0.5<br/>Publisher name: Elsevier  
Source: researchoutputwizard  
Source ID: 5353  
Research output: Contribution to journal > Article > Scientific > peer-review

### Sustainable nutrients recovery and recycling by optimizing the chemical addition sequence for struvite precipitation from raw swine slurries

Livestock farming contributes heavily to nitrogen (N) and phosphorus (P) flows into the environment, a major cause of eutrophication of coastal and freshwater systems. Furthermore, the growing demand for N-P fertilizers is increasing the emission of anthropogenic reactive N into the atmosphere and the depletion of the current P reserves. Therefore, it is essential to minimize the anthropogenic impact on the environment and recycle the wasted N-P for agricultural reuse. This study focused on enhancing struvite ( $\text{MgNH}_4\text{PO}_4 \cdot 6\text{H}_2\text{O}$ ) precipitation from raw swine slurries in batch and laboratory-scale reactors. Different chemical addition sequences were evaluated, and the best removal efficiency (E%) was obtained when the chemicals were mixed before the precipitation process. Struvite was detected at a pH as low as 6 (E%N-P~50%), and high E%N-P was found at pH 7–9.5 (80–95%). Furthermore, air stripping was used in place of NaOH to adjust pH, returning the same efficiency as if only alkali had been used. XRD and FE-SEM analysis of the precipitate showed that the recovered struvite was of high purity with orthorhombic crystalline structure and only trace amounts of impurities from matrix organics, co-precipitation products (CaO and amorphous calcium-phosphates), and residuals of added chemicals (MgO).

#### General information

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Department of Chemistry and Bioengineering, Department of Materials Science  
Contributors: Taddeo, R., Kolppo, K., Lepistö, R.  
Number of pages: 7  
Pages: 52-58  
Publication date: 15 Sep 2016  
Peer-reviewed: Yes

#### Publication information

Journal: Journal of Environmental Management

Volume: 180  
ISSN (Print): 0301-4797  
Ratings:

Scopus rating (2016): CiteScore 5.9 SJR 1.161 SNIP 1.833

Original language: English

ASJC Scopus subject areas: Environmental Engineering, Waste Management and Disposal, Management, Monitoring, Policy and Law

Keywords: Air stripping, Chemical addition, Crystallization, Manure management, Nutrients recycling, Struvite  
DOIs:

10.1016/j.jenvman.2016.05.009

Source: Scopus

Source ID: 84978733912

Research output: Contribution to journal > Article > Scientific > peer-review

### **Synthesis, crystal structure, spectral, dielectric characteristics and conduction mechanism of two novel carboxylates of 1-benzhydrylpiperazine**

Two new 1-benzhydrylpiperazinium carboxylates with tartrate and maleate, (C<sub>17</sub>H<sub>21</sub>N<sub>2</sub>)(C<sub>4</sub>H<sub>5</sub>O<sub>6</sub>) and (C<sub>17</sub>H<sub>22</sub>N<sub>2</sub>)(C<sub>4</sub>H<sub>3</sub>O<sub>4</sub>)<sub>2</sub>, have been synthesized and characterized. Crystal structure determinations show that the compounds crystallize in the P2<sub>1</sub> and the P2<sub>1</sub>/c space groups of the monoclinic system, respectively. Only in the maleate the organic group is protonated on both nitrogen atoms of piperazine ring. The infrared spectra of these compounds reported from 400 to 4000 cm<sup>-1</sup> confirmed the presence of the principal bands assigned to the internal modes of cations and anions of both compounds. The optical band gaps were calculated and found to be 3.46 and 4.14 eV for tartrate and maleate, respectively. Different molecular motions were determinate via dielectric relaxation spectroscopy. Measurements of AC conductivity as a function of frequency at different temperatures indicated the hopping conduction mechanism. The number of <sup>13</sup>C CP-MAS NMR lines is in good agreement with the crystallographic data. Graphical abstract: [Figure not available: see fulltext.]

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Laboratory of Chemical Materials, Faculty of Sciences of Bizerte, Carthage University

Contributors: Wacharine, I., Valkonen, A., Rzaigui, M., Smirani, W.

Number of pages: 14

Pages: 2007-2020

Publication date: 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Monatshefte fur Chemie

Volume: 146

Issue number: 12

ISSN (Print): 0026-9247

Ratings:

Scopus rating (2015): CiteScore 2.2 SJR 0.33 SNIP 0.561

Original language: English

ASJC Scopus subject areas: Chemistry(all)

Keywords: Carboxylic acids, Crystal structure, Hydrogen bonds, NMR spectroscopy, Solid state, X-ray structure determination

DOIs:

10.1007/s00706-015-1553-1

URLs:

<http://www.scopus.com/inward/record.url?scp=84939509914&partnerID=8YFLogxK> (Link to publication in Scopus)

Research output: Contribution to journal > Article > Scientific > peer-review

### **Tailored Fabrication of Transferable and Hollow Weblike Titanium Dioxide Structures**

The preparation of weblike titanium dioxide thin films by atomic layer deposition on cellulose biotemplates is reported. The method produces a TiO<sub>2</sub> web, which is flexible and transferable from the deposition substrate to that of the end application. Removal of the cellulose template by calcination converts the amorphous titania to crystalline anatase and gives the structure a hollow morphology. The TiO<sub>2</sub> webs are thoroughly characterized using electron microscopy, X-ray diffraction, and X-ray photoelectron spectroscopy to give new insight into manufacturing of porous titanium dioxide structures by means of template-based methods. Functionality and integrity of the TiO<sub>2</sub> hollow weblike thin films were successfully confirmed by applying them as electrodes in dye-sensitized solar cells.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Research group: Chemistry & Advanced Materials, Optoelectronics Research Centre, Research group: Surface Science, Department of Materials Science, Research group: Plastics and Elastomer Technology

Contributors: Hiltunen, A., Lahtonen, K., Saari, J., Ojanperä, A., Sarlin, E., Wondraczek, H., Efimov, A., Kaunisto, K., Vivo, P., Maccato, C., Barreca, D., Fardim, P., Tkachenko, N., Valden, M., Lemmetyinen, H.

Number of pages: 8

Pages: 64-71

Publication date: 2017

Peer-reviewed: Yes

Early online date: 16 Nov 2016

### Publication information

Journal: ChemPhysChem

Volume: 18

ISSN (Print): 1439-4235

Ratings:

Scopus rating (2017): CiteScore 5.5 SJR 1.28 SNIP 0.781

Original language: English

DOIs:

10.1002/cphc.201600930

### Bibliographical note

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Source: PubMed

Source ID: 27805802

Research output: Contribution to journal > Article > Scientific > peer-review

### Techno-economic analysis of four concepts for thermal decomposition of methane: Reduction of CO<sub>2</sub> emissions in natural gas combustion

This paper presents a techno-economic analysis of four concepts that apply the thermal decomposition of methane (TDM) with the aim of reducing carbon dioxide emissions in natural gas combustion. Different technical solutions are applied to convert methane in natural gas to gaseous hydrogen, which is combusted to produce electricity with a steam power cycle, and solid carbon, which is assumed to be sold as carbon black. The cost of electricity production and the potential to reduce CO<sub>2</sub> emissions in each concept were evaluated and compared to the reference case of direct methane combustion. With a moderate emission allowance price (20 €/t<sub>CO<sub>2</sub></sub>) and product carbon price (500 €/t<sub>carbon</sub>) the cost of electricity production in the concepts was 12–58% higher than in the reference case. However, the price of product carbon had a significant effect on the feasibility of the concepts. Thus, the methane burner, which showed the best performance, produced 17% less CO<sub>2</sub> emissions per MWh<sub>e</sub> and had a smaller cost of electricity production than the reference case already with the carbon price of 600–700 €/t<sub>carbon</sub>.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Power Plant and Combustion Technology, ÅF-Consult Oy

Contributors: Keipi, T., Hankalin, V., Nummelin, J., Raiko, R.

Pages: 1-12

Publication date: 2016

Peer-reviewed: Yes

Early online date: 2015

### Publication information

Journal: Energy Conversion and Management

Volume: 110

ISSN (Print): 0196-8904

Ratings:

Scopus rating (2016): CiteScore 9.3 SJR 2.232 SNIP 2.107

Original language: English

Keywords: Carbon capture, Natural gas, Carbon black, Methane decomposition, Techno-economic analysis, Carbon dioxide

DOIs:

10.1016/j.enconman.2015.11.057

## The effect of flame treatment on surface properties and heat sealability of low-density polyethylene coating

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Energy and Process Engineering, Engineering materials science and solutions (EMASS)

Contributors: Tuominen, M., Ek, M., Saloranta, P., Toivakka, M., Kuusipalo, J.

Pages: 201-214

Publication date: 2013

Peer-reviewed: Yes

### Publication information

Journal: Packaging Technology and Science

Volume: 26

Issue number: 4

ISSN (Print): 0894-3214

Ratings:

Scopus rating (2013): CiteScore 2.5 SJR 0.713 SNIP 1.31

Original language: English

DOIs:

10.1002/pts.1975

### Bibliographical note

Article first published online: 14 May 2012 : Poistettu tupla r=1325 portfolio13<br/>Contribution:

organisation=epr,FACT1=1<br/>Publisher name: John Wiley & Sons

Source: researchoutputwizard

Source ID: 3580

Research output: Contribution to journal › Article › Scientific › peer-review

## The Effect of Phosphorus Exposure on Diesel Oxidation Catalysts-Part I: Activity Measurements, Elementary and Surface Analyses

The effects of phosphorus poisoning on the activity of PtPd and Pt diesel oxidation catalysts and on the activity of the support material were investigated using the gas phase laboratory-scale-aging procedure. The catalysts were treated using two different phosphorus concentrations (0.065 and 0.13 mol/L (NH<sub>4</sub>)<sub>2</sub>HPO<sub>4</sub>). The deactivation was studied by inductively coupled plasma optical emission spectroscopy, electron microscopy, X-ray diffractometry, X-ray photoelectron spectrometry and Fourier-transform infrared reflectance, N<sub>2</sub>-physisorption, and activity measurements with CO, C<sub>3</sub>H<sub>6</sub> and NO. The amount of accumulated phosphorus was higher on the Pt catalyst surface than on the PtPd catalyst and significantly higher on the surface of the bare support material. Phosphorus concentration was uniform throughout the support layer (down to the 10 μm), and phosphorus was found as phosphate, although it can also form compounds like AlPO<sub>4</sub> with the support. The treatment with low phosphorus concentration was found to have a clear deactivation effect only for C<sub>3</sub>H<sub>6</sub> oxidation activity on PtPd catalysts above 200 degrees C. The treatment with high phosphorus concentration significantly decreased the activity of both the PtPd and Pt catalysts. In particular, the C<sub>3</sub>H<sub>6</sub> and NO oxidation activities of the fresh and P-treated Pt catalysts were higher than those of the PtPd catalysts for the entire temperature range.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Materials Characterization, Univ Oulu, University of Oulu, Fac Technol, Environm & Chem Engn, Aalto University, Dinex Ecocat Oy, Catalyst Res

Contributors: Kärkkäinen, M., Kolli, T., Honkanen, M., Heikkinen, O., Huuhtanen, M., Kallinen, K., Lepistö, T., Lahtinen, J., Vippola, M., Keiski, R. L.

Number of pages: 10

Pages: 961-970

Publication date: Oct 2015

Peer-reviewed: Yes

### Publication information

Journal: Topics in Catalysis

Volume: 58

Issue number: 14

ISSN (Print): 1022-5528

Ratings:

Scopus rating (2015): CiteScore 4.7 SJR 0.926 SNIP 0.777

Original language: English

Keywords: Phosphorus, Deactivation, Poisoning, Diesel oxidation catalyst, Platinum, Palladium, NO OXIDATION, THERMAL-STABILITY, DEACTIVATION, REDUCTION, MECHANISMS, BEHAVIOR, EXHAUST

DOIs:

10.1007/s11244-015-0464-z

Source: WOS

Source ID: 000362581900016

Research output: Contribution to journal › Article › Scientific › peer-review

### **The Effect of Phosphorus Exposure on Diesel Oxidation Catalysts-Part II: Characterization of Structural Changes by Transmission Electron Microscopy**

Phosphorus poisoning and its effect on the diesel oxidation catalysts morphology was studied by transmission electron microscopy (TEM). The studied catalyst samples were PtPd or Pt supported on the alumina-based washcoat including additives. The laboratory-scale phosphorus exposures were carried out with two different phosphorus concentrations. The cross-sectional TEM samples were prepared from the fresh and phosphorus-treated catalysts. After phosphorus exposures, significant structural changes were observed compared to the fresh catalysts. The shape of the noble metal particles had changed from irregular to more spherical-shaped particles. In addition, phosphorus was detected throughout the catalyst TEM samples but the amount varied depending on the local composition of the support. Phosphorus accumulated mainly in the alumina-containing areas of the support and indications of dense and amorphous aluminium phosphates were found. Based on the results gained, cross-sectional TEM characterization is essential to observe these kinds of morphological changes in the catalysts caused e.g. by phosphorus exposures. In addition, cross-sectional TEM samples are needed to study the effect of local variation in the support composition on the phosphorus accumulation.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Materials Characterization, Univ Oulu, University of Oulu, Fac Technol Mass & Heat Transfer Proc Engn, Aalto University, Dinex Ecocat Oy

Contributors: Honkanen, M., Kärkkäinen, M., Heikkinen, O., Kallinen, K., Kolli, T., Huuhtanen, M., Lahtinen, J., Keiski, R. L., Lepistö, T., Vippola, M.

Number of pages: 6

Pages: 971-976

Publication date: Oct 2015

Peer-reviewed: Yes

#### **Publication information**

Journal: Topics in Catalysis

Volume: 58

Issue number: 14

ISSN (Print): 1022-5528

Ratings:

Scopus rating (2015): CiteScore 4.7 SJR 0.926 SNIP 0.777

Original language: English

Keywords: Diesel oxidation catalyst, Phosphorus poisoning, Structural characterization, Transmission electron microscopy, 3-WAY CATALYST, DEACTIVATION, MECHANISMS, EXHAUST, IMPACT

Electronic versions:

Honkanen et al\_accepted manuscript

DOIs:

10.1007/s11244-015-0465-y

URLs:

<http://urn.fi/URN:NBN:fi:tty-201710182015>

Source: WOS

Source ID: 000362581900017

Research output: Contribution to journal › Article › Scientific › peer-review

### **The effect of the outermost fibre layers on solubility of dissolving grade pulp**

Dissolving pulps are used to manufacture various cellulose derived products through cellulose dissolution. Solubility of cellulose pulp has been claimed to be strongly dependent on the porosity development, the degree of polymerisation and the pulp viscosity. The removal of external cell walls has been proposed to have a key role in the pulp solubility. In this paper, the effect of the outermost surface layers on the solubility of a dissolving grade pulp was studied. Furthermore the effect of mechanical peeling and combined mechanical and enzymatic treatment on pulp solubility was compared. Based on the results combined mechanical and enzymatic treatment efficiently opens up the fibre structure and has a clear positive effect on the solubility of dissolving pulp. It seems that long fibre fraction is less accessible to solvent chemicals

than the other pulp fractions. Mechanical peeling of outer fibre layers does not improve fibre dissolution to NaOH/ZnO. Thus, it seems that peeling alone is not a sufficient pre-treatment prior to dissolution. The results also revealed that the peeling treatment does not enhance the effects of enzymes as the studied mechanical treatment does.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Materials Science, Research group: Fibre Materials, Department of Forest Products Technology, VTT Technical Research Centre of Finland, Latvian State Institute of Wood Chemistry, Aalto University

Contributors: Grönqvist, S., Treimanis, A., Kämpuri, T., Maloney, T., Skute, M., Grinfelds, U., Vehviläinen, M., Suurnäkki, A.

Number of pages: 11

Pages: 3955-3965

Publication date: 2015

Peer-reviewed: Yes

#### Publication information

Journal: Cellulose

Volume: 22

Issue number: 6

ISSN (Print): 0969-0239

Ratings:

Scopus rating (2015): CiteScore 5.2 SJR 1.122 SNIP 1.202

Original language: English

ASJC Scopus subject areas: Polymers and Plastics

Keywords: Cellulose dissolution, Dissolving pulp, Enzymatic hydrolysis, Hydromechanical peeling, Porosity, Solute exclusion

DOIs:

10.1007/s10570-015-0709-9

URLs:

<http://www.scopus.com/inward/record.url?scp=84941357236&partnerID=8YFLogxK> (Link to publication in Scopus)

Source: Scopus

Source ID: 84946490244

Research output: Contribution to journal > Article > Scientific > peer-review

#### The effects of UV irradiation to polyetheretherketone fibres: Characterization by different techniques

The effects of UV irradiation on polyetheretherketone (PEEK) fibres were investigated in this study. PEEK fibres were manufactured with a melt spinning system and then artificially aged with simulated solar UV light. Fibres were then characterized by mechanical tests, Fourier transform infrared spectroscopy (FTIR), differential scanning calorimetry (DSC), rheology, thermogravimetric analysis (TGA) and scanning electron microscopy (SEM). PEEK, best known for its excellent thermal stability, suffered greatly from the effects of UV irradiation. The low UV stability manifested as embrittlement of the fibres in the mechanical tests, increased crosslinking rate in the rheological tests, formation of carbonyl and hydroxyl groups and changes in the nature of the carbon-hydrogen bonds in the FTIR, diminished thermal properties in TGA, and transverse cracks in the SEM photos. DSC was found to be an inaccurate technique for estimating the degradation level of PEEK fibres, whereas the carbonyl index measured by FTIR was found to be the most convenient technique. © 2014 Elsevier Ltd. All rights reserved.

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Tampere University of Technology

Contributors: Mylläri, V., Ruoko, T. P., Järvelä, P.

Number of pages: 7

Pages: 278-284

Publication date: 2014

Peer-reviewed: Yes

#### Publication information

Journal: Polymer Degradation and Stability

Volume: 109

ISSN (Print): 0141-3910

Ratings:

Scopus rating (2014): CiteScore 4.9 SJR 1.282 SNIP 1.889

Original language: English

ASJC Scopus subject areas: Polymers and Plastics, Materials Chemistry, Mechanics of Materials, Condensed Matter Physics

Keywords: PEEK, Fibre, Ultraviolet, Rheology, POLY(ETHER ETHER KETONE), STRUCTURE/DEGRADABILITY RELATIONSHIPS, SCANNING CALORIMETRY, THERMAL-DEGRADATION, POLYPROPYLENE, PHOTODEGRADATION, POLYMERS, PHOTOOXIDATION, CRYSTALLINITY

Electronic versions:

The\_effects\_of\_UV\_irradiation\_pre-print

DOIs:

10.1016/j.polymdegradstab.2014.08.003

URLs:

<http://urn.fi/URN:NBN:fi:tty-201612024839>

URLs:

<http://www.scopus.com/inward/record.url?scp=84907310748&partnerID=8YFLogxK> (Link to publication in Scopus)

### Bibliographical note

Contribution: organisation=mol,FACT1=0.8  
Contribution: organisation=keb,FACT2=0.2  
Portfolio EDEND: 2014-09-10  
Publisher name: Elsevier Ltd

Source: researchoutputwizard

Source ID: 1117

Research output: Contribution to journal › Article › Scientific › peer-review

### Thermo-catalytic decomposition of methane: The effect of reaction parameters on process design and the utilization possibilities of the produced carbon

The study presents a path for selecting the reaction and reactor parameters of a process applying thermo-catalytic decomposition of methane (TDM). Temperature and catalyst are the main reaction parameters affecting the type of TDM carbon and defining the reaction's theoretical heat requirement. Secondly, the reaction parameters affect the reactor design including the selection of reactor type and heating source as well as the reactor dimensioning. The reactor dimensioning is discussed by highlighting the methane residence time requirement at different reaction conditions. Finally, the economic value of the TDM products is analyzed. According to the analyses, the reaction temperature and catalyst have a significant effect on reactor design and on the value and utilization possibilities of the TDM carbon. The prices of carbon products vary greatly as does the global demand of those. The utilization possibilities of carbon highly affect the overall viability of the TDM process and therefore should be carefully considered during process design.

### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Chemistry and Bioengineering, Research group: Power Plant and Combustion Technology

Contributors: Keipi, T., Tolvanen, K. E., Tolvanen, H., Konttinen, J.

Number of pages: 12

Pages: 923-934

Publication date: Oct 2016

Peer-reviewed: Yes

### Publication information

Journal: Energy Conversion and Management

Volume: 126

ISSN (Print): 0196-8904

Ratings:

Scopus rating (2016): CiteScore 9.3 SJR 2.232 SNIP 2.107

Original language: English

Keywords: Carbon capture, Process design, Natural gas, Methane decomposition, Hydrogen production

DOIs:

10.1016/j.enconman.2016.08.060

Research output: Contribution to journal › Article › Scientific › peer-review

### Top layer coatability on barrier coatings

#### General information

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Energy and Process Engineering

Contributors: Bollström, R., Tuominen, M., Määtänen, A., Peltonen, J., Toivakka, M.



Pages: 26-32  
Publication date: 2012  
Peer-reviewed: Yes

#### **Publication information**

Journal: Progress in Organic Coatings  
Volume: 73  
Issue number: 1  
ISSN (Print): 0300-9440  
Ratings:  
Scopus rating (2012): CiteScore 3.6 SJR 1.048 SNIP 1.805  
Original language: English  
DOIs:  
10.1016/j.porgcoat.2011.08.015  
URLs:  
<http://www.elsevier.com/locate/porgcoat>

#### **Bibliographical note**

Contribution: organisation=epr pap,FACT1=1<br/>Publisher name: Elsevier BV  
Source: researchoutputwizard  
Source ID: 3933  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Toward more controlled, nanoscale barrier layers in packaging**

#### **General information**

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Department of Energy and Process Engineering  
Contributors: Lahtinen, K., Johansson, P., Kääriäinen, T., Maydannik, P., Cameron, D., Kuusipalo, J.  
Number of pages: 3  
Pages: 1-3  
Publication date: 2012  
Peer-reviewed: Yes

#### **Publication information**

Journal: Plastics Research Online  
Issue number: 17th August  
Original language: English  
DOIs:  
10.2417/spepro.004237

#### **Bibliographical note**

17 August 2012. ei ut-numeroa 20.8.2013<br/>Contribution: organisation=epr,FACT1=1<br/>Publisher name: Society of Plastics Engineers (SPE)  
Source: researchoutputwizard  
Source ID: 4623  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Utilisation of continuous atomic layer deposition process for barrier enhancement of extrusion-coated paper**

#### **General information**

Publication status: Published  
MoE publication type: A1 Journal article-refereed  
Organisations: Department of Energy and Process Engineering, Engineering materials science and solutions (EMASS)  
Contributors: Lahtinen, K., Maydannik, P., Johansson, P., Kääriäinen, T., Cameron, D. C., Kuusipalo, J.  
Pages: 3916-3922  
Publication date: 2011  
Peer-reviewed: Yes

#### **Publication information**

Journal: Surface and Coatings Technology  
Volume: 205  
Issue number: 15

ISSN (Print): 0257-8972

Ratings:

Scopus rating (2011): CiteScore 3.7 SJR 1.041 SNIP 1.841

Original language: English

DOIs:

10.1016/j.surfcoat.2011.02.009

#### **Bibliographical note**

Contribution: organisation=epr pap,FACT1=1

Source: researchoutputwizard

Source ID: 6531

Research output: Contribution to journal › Article › Scientific › peer-review

#### **Valorization of Finnish mining tailings for use in the ceramics industry**

The present study valorized Finnish mining tailings waste to identify opportunities for the use of ceramics technologies. On the basis of their mineralogical and chemical contents, the five selected tailings wastes represented felsic mining tailings (FMT) rich in quartz and alkali feldspars, mining tailings dominated by Mg- and Fe-bearing minerals (MgFeMT), and mining tailings rich in carbonate minerals (CMT). Preliminary pilot studies indicated that the FMT materials are potential secondary raw materials for mullite-type ceramics. An Al additive was needed, since the Al<sub>2</sub>O<sub>3</sub> content of the studied tailings was too low for mullitization. In addition, carbonate-bearing tailings with Ca silicates can be applicable for chemically bonded phosphate ceramic (CBPC) synthesis. Based on a literature review, FMT are viable source materials for the production of geopolymers, but a high initial Si:Al ratio (in quartz-rich FMT) may lead to partial geopolymerization. Preliminary results from the geopolymerization of pre-heated phlogopite mica mixed with metakaolin gave promising findings, with the formation of a geopolymer having good compressive strength. The findings support the viability of MgFeMT materials rich in phlogopite mica for the production of alkali-activated ceramics.

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Materials Science, Research group: Ceramic materials, Geological Survey of Finland, VTT, Geologian tutkimuskeskus, University of Oulu

Contributors: Solismaa, S., Ismailov, A., Karhu, M., Sreenivasan, H., Lehtonen, M., Kinnunen, P., Illikainen, M., Räisänen, M.

Pages: 33-54

Publication date: 2018

Peer-reviewed: Yes

#### **Publication information**

Journal: BULLETIN OF THE GEOLOGICAL SOCIETY OF FINLAND

Volume: 90

Issue number: 1

ISSN (Print): 0367-5211

Ratings:

Scopus rating (2018): CiteScore 1 SJR 0.244 SNIP 0.376

Original language: English

DOIs:

10.17741/bgsf/90.1.002

Research output: Contribution to journal › Article › Scientific › peer-review

#### **Wettability conversion on the liquid flame spray generated superhydrophobic TiO<sub>2</sub> nanoparticle coating on paper and board by photocatalytic decomposition of spontaneously accumulated carbonaceous overlayer**

#### **General information**

Publication status: Published

MoE publication type: A1 Journal article-refereed

Organisations: Department of Energy and Process Engineering, Department of Physics, Engineering materials science and solutions (EMASS)

Contributors: Teisala, H., Tuominen, M., Stepien, M., Haapanen, J., Mäkelä, J. M., Saarinen, J. J., Toivakka, M., Kuusipalo, J.

Pages: 391-408

Publication date: 2013

Peer-reviewed: Yes

#### **Publication information**

Journal: Cellulose  
Volume: 20  
Issue number: 1  
ISSN (Print): 0969-0239  
Ratings:

Scopus rating (2013): CiteScore 5 SJR 1.126 SNIP 1.476  
Original language: English  
DOIs:  
10.1007/s10570-012-9825-y

#### **Bibliographical note**

Published online: 22 November 2012  
Contribution: organisation=epr,FACT1=0.5  
Contribution: organisation=fys,FACT2=0.5  
Publisher name: Springer  
Source: researchoutputwizard  
Source ID: 3526  
Research output: [Contribution to journal](#) › [Article](#) › [Scientific](#) › [peer-review](#)

### **Influence of Atmospheric Plasma Treatment on Surface Properties and Inkjet Printability of Plastic Packaging Film**

#### **General information**

Publication status: Published  
MoE publication type: A3 Part of a book or another research book  
Organisations: Department of Energy and Process Engineering  
Contributors: Lahti, J., Eiroma, K., Tenhunen, T., Pykönen, M., Toivakka, M.  
Pages: 197-203  
Publication date: 2010

#### **Host publication information**

Title of host publication: Advances in Printing and Media Technology  
Editors: Enlund, N., Lovrecek, M.  
ISBN (Print): 978-3-9812704-2-6

#### **Bibliographical note**

Contribution: organisation=epr pap,FACT1=1  
Source: researchoutputwizard  
Source ID: 8549  
Research output: [Chapter in Book/Report/Conference proceeding](#) › [Chapter](#) › [Scientific](#) › [peer-review](#)

### **The name of the thesis: Atmospheric Plasma Treatment in Extrusion Coating, Topic: The Effect of Flame Treatment on the Sealability of Extrusion Coated Paper**

#### **General information**

Publication status: Published  
MoE publication type: A3 Part of a book or another research book  
Organisations: Department of Energy and Process Engineering  
Contributors: Tuominen, M.  
Number of pages: 5  
Pages: 1-5  
Publication date: 2011

#### **Host publication information**

Title of host publication: PaPSaT, International Doctoral Programme in Pulp and Paper Science and Technology in Finland, Yearbook 2011  
Place of publication: Espoo  
Publisher: Aalto University School of science and technology  
Editor: Kärkkäinen, S.

#### **Bibliographical note**

Contribution: organisation=epr pap,FACT1=1  
Source: researchoutputwizard  
Source ID: 7421  
Research output: [Chapter in Book/Report/Conference proceeding](#) › [Chapter](#) › [Scientific](#) › [peer-review](#)

**The name of the thesis: Surface Treatment in Extrusion Coating, Topic: The Influence of Corona and Flame Treatment on Sealability of Extrusion Coated Paper**

**General information**

Publication status: Published  
MoE publication type: A3 Part of a book or another research book  
Organisations: Department of Energy and Process Engineering  
Contributors: Tuominen, M.  
Number of pages: 5  
Pages: 1-5  
Publication date: 2010

**Host publication information**

Title of host publication: PaPSaT, International Doctoral Programme in Pulp and Paper Science and Technology in Finland, Yearbook 2010  
Editor: Kärkkäinen, S.

**Bibliographical note**

Contribution: organisation=epr,pap,FACT1=1  
Source: researchoutputwizard  
Source ID: 9444  
Research output: Chapter in Book/Report/Conference proceeding › Chapter › Scientific › peer-review

**Atomic layer deposition process for barrier applications of flexible packaging**

**General information**

Publication status: Published  
MoE publication type: B3 Non-refereed article in conference proceedings  
Organisations: Department of Energy and Process Engineering  
Contributors: Johansson, P., Lahtinen, K., Kuusipalo, J., Kääriäinen, T., Maydannik, P., Cameron, D.  
Number of pages: 12  
Pages: 1-12  
Publication date: 2010

**Host publication information**

Title of host publication: TAPPI 2010 PLACE Conference, April 18-21, 2010, Albuquerque NM, USA

**Bibliographical note**

Contribution: organisation=epr,FACT1=1  
Source: researchoutputwizard  
Source ID: 8216  
Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific

**Deposition of flame synthesised nanoparticles on paperboard surface**

**General information**

Publication status: Published  
MoE publication type: B3 Non-refereed article in conference proceedings  
Organisations: Research area: Aerosol Physics, Department of Physics, Department of Energy and Process Engineering  
Contributors: Aromaa, M., Haapanen, J., Teisala, H., Tuominen, M., Kuusipalo, J., Stepien, M., Saarinen, J., Toivakka, M., Mäkelä, J.  
Pages: 17-17  
Publication date: 2011

**Host publication information**

Title of host publication: NOSA & FAAR 2011, Nordic Aerosol Symposium, November 9-11, 2011, Tampere, Finland  
Place of publication: Tampere  
Publisher: Nordic Society for Aerosol Research

**Publication series**

Name: Nordic Aerosol Symposium NOSA & FAAR  
Publisher: Nordic Society for Aerosol Research

**Bibliographical note**

ei ut-numeroa 26.10.2013  
Contribution: organisation=fys,FACT1=0.5  
Contribution: organisation=epr,pap,FACT2=0.5

Source: researchoutputwizard

Source ID: 5723

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific

### **Diffusion of acidic solution through rubber at high temperature and its effect on metal-rubber interface degradation**

#### **General information**

Publication status: Published

MoE publication type: B3 Non-refereed article in conference proceedings

Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Teknikum Oy, Outotec Research Center, Laboratory of Polymer Technology, Centre of Excellence in Functional Materials at Biological Interfaces, Åbo Akademi University

Contributors: Sarlin, E., Rosling, A., Mustakangas, M., Laihonen, P., Lindgren, M., Vuorinen, J.

Publication date: 2015

#### **Host publication information**

Title of host publication: Proceedings of SAMPE Europe Conference

ISBN (Electronic): 978-90-821727-3-7

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific

### **Research on icing behavior and ice adhesion testing of icephobic surfaces**

Surface engineering shows potential to provide sustainable approach to icing problems. Currently several passive anti-ice mechanisms adoptable to coatings are known but further research is required to proceed for practical applications. Icing wind tunnel and centrifugal ice adhesion test equipment enable the evaluation and development of anti-ice and icephobic coatings for e.g., wind turbine applications but also other growing players in arctic environment e.g. oil, extractive and logistic industries. This research is focused on the evaluation of icing properties of various surfaces.

#### **General information**

Publication status: Published

MoE publication type: B3 Non-refereed article in conference proceedings

Organisations: Department of Materials Science, Research group: Surface Engineering, Univ Modena & Reggio Emilia, Universita di Modena e Reggio Emilia, Dept Engn Enzo Ferrari

Contributors: Koivuluoto, H., Stenroos, C., Ruohomaa, R., Bolelli, G., Lusvarghi, L., Vuoristo, P.

Number of pages: 6

Pages: 183-188

Publication date: 2015

#### **Host publication information**

Title of host publication: 16th International Workshop on Atmospheric Icing of Structures, IWAIS 2015, June 28-July 3, 2015, Uppsala, Sweden

ISBN (Electronic): 978-91-637-8552-8

URLs:

<http://iwais.org/>

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific

### **Two-component aerosol nanoparticle coating for paperboard on roll-to-roll process**

#### **General information**

Publication status: Published

MoE publication type: B3 Non-refereed article in conference proceedings

Organisations: Research area: Aerosol Physics, Department of Physics, Department of Energy and Process Engineering

Contributors: Haapanen, J., Aromaa, M., Teisala, H., Tuominen, M., Stepien, M., Saarinen, J., Toivakka, M., Kuusipalo, J., Mäkelä, J.

Number of pages: 1

Pages: 1-1

Publication date: 2012

#### **Host publication information**

Title of host publication: EAC-2012 Granada, European Aerosol Conference, 2-7 Sept 2012, Granada, Spain

Publisher: EAA, AECTA

#### **Publication series**

Name: European Aerosol Conference EAC

URLs:

<http://www.eac2012.com/EAC2012Book/>

#### **Bibliographical note**

ei ut-numeroa 13.8.2013<br/>Contribution: organisation=fys,FACT1=0.5<br/>Contribution:

organisation=epr,FACT2=0.5<br/>Publisher name: EAA, AECTA

Source: researchoutputwizard

Source ID: 4117

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific

### **Atmospheric Plasma Treatment of Plastic Packaging Film: Effects on Surface Properties and UV Inkjet Printability**

#### **General information**

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Department of Energy and Process Engineering, Engineering materials science and solutions (EMASS)

Contributors: Lahti, J., Eiroma, K., Tenhunen, T., Pykönen, M., Toivakka, M., Tuominen, M.

Number of pages: 31

Pages: 1-31

Publication date: 2011

#### **Host publication information**

Title of host publication: 13th TAPPI European PLACE Conference, Bregenz, Austria, 30 May - 1 June, 2011

Place of publication: Norcross, GA

Publisher: TAPPI

#### **Publication series**

Name: TAPPI European PLACE Conference

Publisher: TAPPI

URLs:

[http://www.tappi.org/content/events/11EUROPLACE/papers/16\\_1.pdf](http://www.tappi.org/content/events/11EUROPLACE/papers/16_1.pdf)

#### **Bibliographical note**

ei ut-numeroa 29.3.2014<br/>Contribution: organisation=epr,FACT1=1

Source: researchoutputwizard

Source ID: 6528

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

### **Corrosion propagation phase studies on Finnish reinforced concrete facades**

#### **General information**

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Department of Civil Engineering, Research group: Service Life Engineering of Structures, Department of Materials Science, Research group: Materials Characterization

Contributors: Köliö, A., Honkanen, M., Lahdensivu, J.

Publication date: 2015

#### **Host publication information**

Title of host publication: 1st International Symposium on Building Pathology : ISBP 2015

Place of publication: Porto

Publisher: FEUP Edicoes (Faculdade de Engenharia da Universidade do Porto Edicoes)

ISBN (Print): 978-972-752-174-6

#### **Bibliographical note**

ORG=rak,0.5

ORG=mol,0.5

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

### **Design driven world of cellulose-from bulk to luxury?**

Tekes-the Finnish Funding Agency for Innovation has granted funding 4,5 million funding for a project targeting on new approaches for use of wood-based cellulose. Project "Design Driven Value Chains in The World of Cellulose" (DWoC) launched by VTT Technical Research Centre of Finland, Aalto University and Tampere University of Technology integrates design and design processes into the strategic development of businesses operating in the field. The aim is to create a business ecosystem to serve both existing industry and a new, growing cellulose-based industry, and to brand

Finland as a producer of refined, cellulose-based products. This manuscript summarises the future visions and background aspects and facts that have led to the initiation of the project. The presentation based on the manuscript also presents some of the first demonstrator processes and products developed during the first operational year of the project. These demonstrators include: Fibre yarn process that produces yarn from cellulose pulp fibres without traditional spinning process using novel wet extrusion technique (figure on right). Foam forming method for manufacturing well-formed foamed structures for new product applications 3D-printing technology enabling customisable on demand production of fibre structures and components using modified cellulosic raw materials.

#### **General information**

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Engineering materials science and solutions (EMASS), VTT Technical Research Centre of Finland, Aalto University

Contributors: Qvintus, P., Kataja, K., Heikkilä, P., Salmela, J., Lehmonen, J., Ketoja, J., Hänninen, T., Harlin, A., Härkäsalmi, T., Vuorinen, J., Vuorinen, T.

Number of pages: 8

Pages: 67-74

Publication date: 2014

#### **Host publication information**

Title of host publication: Fibre Value Chain Conference and Expo 2014: Pulp and Paper Bioenergy Bioproducts

Publisher: Appita Inc.

ISBN (Print): 9780987168443

ASJC Scopus subject areas: Industrial and Manufacturing Engineering, Energy Engineering and Power Technology, Renewable Energy, Sustainability and the Environment

Keywords: Cellulose, Design, Design driven research, Ecodesign, New business, New cellulose technologies

URLs:

<http://www.scopus.com/inward/record.url?scp=84923271599&partnerID=8YFLogxK> (Link to publication in Scopus)

#### **Bibliographical note**

EXT="Harlin, Ali"

EXT="Heikkilä, Pirjo"

Source: Scopus

Source ID: 84923271599

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

### **Development of sustainable paper coatings using nanoscale industrial**

#### **General information**

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Department of Energy and Process Engineering

Contributors: Markert, F., Breedveld, L., Lahti, J., Vangeneugden, D.

Pages: 80-84

Publication date: 2010

#### **Host publication information**

Title of host publication: i-SUP 2010, Innovation for Sustainable Production, Conference 4, Materials for Sustainable Production, Bruges, Belgium, 18-21 April, 2010

URLs:

<http://www.i-sup2010.org>

#### **Bibliographical note**

Contribution: organisation=epr,FACT1=1

Source: researchoutputwizard

Source ID: 8749

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

### **Effect of Pigment Volume Concentration and Drying Aspects on the Enzyme Activity of Clay Coatings**

#### **General information**

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Department of Energy and Process Engineering

Contributors: Johansson, K., Christophliemk, H., Jönsson, L. J., Järnström, L.

Pages: 129-143  
Publication date: 2010

#### Host publication information

Title of host publication: 11th Advanced Coating Fundamentals Symposium Proceedings, The Latest Advances in Coating Research and Development, 11-13 October 2010, Munich, Germany  
Place of publication: USA  
Publisher: TAPPI Press  
ISBN (Print): 1-59510-203-5

#### Publication series

Name: TAPPI Advanced Coating Fundamentals Symposium  
Publisher: TAPPI PRESS

#### Bibliographical note

Vuoden 2010 konf.<br/>Contribution: organisation=epr,FACT1=1  
Source: researchoutputwizard  
Source ID: 8215

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

### Flame deposition of superhydrophobic and superhydrophilic nanoparticle coating on paperboard materials

#### General information

Publication status: Published  
MoE publication type: A4 Article in a conference publication  
Organisations: Department of Physics, Department of Energy and Process Engineering, Engineering materials science and solutions (EMASS)  
Contributors: Aromaa, M., Haapanen, J., Teisala, H., Tuominen, M., Kuusipalo, J., Stepien, M., Saarinen, J., Toivakka, M., Mäkelä, J. M.  
Pages: 365-367  
Publication date: 2012

#### Host publication information

Title of host publication: Nanotechnology 2012: Advanced Materials, CNTs, Particles, Films and Composites - 2012 NSTI Nanotechnology Conference and Expo, NSTI-Nanotech 2012, Santa Clara, CA, USA, 18-21 June 2012  
Publisher: Nano Science and Technology Institute NSTI  
ISBN (Print): 978-1-4665-6274-5

#### Publication series

Name: Nanotechnology Conference and Expo Nanotech

#### Bibliographical note

ei ut-numeroa 9.8.2013<br/>Contribution: organisation=fys,FACT1=0.5<br/>Contribution: organisation=epr,FACT2=0.5<br/>Publisher name: Nano Science and Technology Institute NSTI  
Source: researchoutputwizard  
Source ID: 3865

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

### High performance wear and corrosion resistant coatings by novel cladding techniques

In the field of surface engineering, cladding or overlay welding is a group of coating methods used in manufacturing fusion-bonded thick metallic and metal matrix composite (MMC) coatings on a wide variety of metallic base materials with varying degree of deposition rate, dilution and heat input. Growing demands for more material-, energy- and cost-effective overlay welding processes as well as sustainable solutions for performance-critical applications have boosted to develop methods that are capable of producing low diluted and fusion-bonded single layer coatings with high deposition rates. Such novel cladding methods include for instance laser-based high power laser cladding, coaxial hot-wire laser cladding, laser-arc hybrid cladding, non-laser-based Cold Metal Transfer (CMT) cladding and methods that utilize high intensity infrared (IR) light. This paper introduces some of such highly innovative cladding techniques and highlights some microstructural and geometrical features, abrasion and sliding wear, and wet corrosion properties of Fe-, Ni- and Co-based metallic coatings manufactured by novel laser and CMT cladding methods. The research results evidence that with the choice of optimal processing parameters, novel cladding techniques are capable of manufacturing high performance weld overlays with the properties equivalent or near to corresponding wrought alloys and reference overlays with net deposition rates of approximately 5 kg/h and more. Overall, the presented work suggests that discussed methods have high potential in surfacing of new and remanufacturing of service-damaged surfaces in high value components, in building up complex features on existing components and also in near net shape additive manufacturing of functional 3D objects.



### General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Department of Materials Science, Research group: Surface Engineering, Research group: Materials Characterization, Department of Mechanical Engineering and Industrial Systems, Research area: Manufacturing and Automation, Technology Centre Ketek Ltd.

Contributors: Tuominen, J., Näkki, J., Pajukoski, H., Nyssönen, T., Ristonen, T., Peltola, T., Vuoristo, P.

Number of pages: 13

Pages: 105-117

Publication date: Jan 2015

### Host publication information

Title of host publication: Surface Modification Technologies XXVIII : Proceedings of the 28th International Conference on Surface Modification Technologies

Publisher: Valardocs

Editors: Sudarshan, T., Vuoristo, P., Koivuluoto, H.

ISBN (Electronic): 978-81-926196-1-3

Keywords: Cladding, Additive manufacturing, Laser, CMT, Metallien 3D-tulostus, 3D printing, Remanufacturing, Uudelleenvalmistus, Digital manufacturing, Digitaalinen valmistus

### Bibliographical note

koa ei tarkistettu

EXT="Näkki, J."

ORG=mol,0.5

ORG=mei,0.5

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

## Image based measurement of particle phase reynolds stresses in a laboratory scale circulating fluidized bed

### General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Department of Energy and Process Engineering

Contributors: Peltola, J., Kallio, S., Honkanen, M., Saarenrinne, P.

Number of pages: 9

Pages: 1-9

Publication date: 2010

### Host publication information

Title of host publication: 7th International Conference on Multiphase Flow ICMF2010, May 30 - June 4, 2010, Tampa, Florida

URLs:

<http://conferences.dce.ufl.edu/ICMF2010/>

### Bibliographical note

Contribution: organisation=epr,FACT1=1

Source: researchoutputwizard

Source ID: 8965

Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

## Nanoscale surface processing of extrusion coated substrates and plastic films with atmospheric plasma activation and deposition

### General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Department of Materials Science, Engineering materials science and solutions (EMASS)

Contributors: Lahti, J., Lavonen, J.

Pages: 588-600

Publication date: 2012

### Host publication information

Title of host publication: TAPPI PLACE Conference 2012, Helping Me Do My Job Better, Seattle, Washington, USA, 6-9 May 2012

Publisher: TAPPI Press; Curran Associates, Inc

ISBN (Print): 978-1-62276-841-7

#### Publication series

Name: TAPPI PLACE Conference

#### Bibliographical note

Contribution: organisation=mol,FACT1=1<br/>Portfolio EDEND: 2013-12-29<br/>Publisher name: TAPPI Press; Curran Associates, Inc

Source: researchoutputwizard

Source ID: 4622

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

### Nanoscale Surface Processing of Extrusion Coated Substrates and Plastic Films with Atmospheric Plasma Activation and Deposition

#### General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Department of Energy and Process Engineering, Engineering materials science and solutions (EMASS)

Contributors: Lahti, J., Lavonen, J.

Pages: 29-30

Publication date: 2011

#### Host publication information

Title of host publication: Novel nanostructured polymeric materials for food packaging and beyond, International COST Workshop, Espoo, Finland, September 15-16, 2011. VTT Symposium

Place of publication: Espoo

Publisher: VTT

Editor: Vähä-Nissi, M.

ISBN (Print): 978-951-38-7604-3

#### Publication series

Name: International COST Workshop

Publisher: VTT

Volume: 270

ISSN (Print): 0357-9387

#### Bibliographical note

poistettu tupla r=1647<br/>Contribution: organisation=epr pap,FACT1=1

Source: researchoutputwizard

Source ID: 6529

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

### Simulation of ash-forming compounds in the kraft recovery boiler

This paper presents a summary of the doctoral dissertation titled "Modeling Fume Particle Dynamics and Deposition with Alkali Metal Chemistry in Kraft Recovery Boilers". In the thesis, a computational model was developed and used to simulate the behavior of alkali metal compounds in kraft recovery boilers. The model combines, for the first time, the methods of CFD (Computational Fluid Dynamics), equilibrium chemistry, and fine particle dynamics to model the formation and deposition of fume particles. Fume particles are below 1 µm in diameter and form through the condensation of the alkali metal compounds. The model has been partially validated in an operating recovery boiler in terms of fume particle composition, but the modeling results also shed light on processes that cannot be investigated through experimental methods alone. For example, the modeling results indicate that thermophoresis is the main factor leading to fume deposit formation.

#### General information

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Department of Chemistry and Bioengineering, Research group: Power Plant and Combustion Technology

Contributors: Leppänen, A., Välimäki, E., Oksanen, A.

Number of pages: 10

Publication date: 2015

#### Host publication information

Title of host publication: 10th European Conference on Industrial Furnaces and Boilers

Place of publication: Porto, Portugal

ISBN (Electronic): 978-972-99309-7-3

Keywords: kraft recovery boiler, alkali metal, fine particle, deposition, computational fluid dynamics

URLs:

<http://www.cenertec.pt/infub/>

Source: Bibtex

Source ID: urn:c88098f51c0b1f0404f1a0f11bbb345f

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

### **Solution Modified Fumed Silica and Its Effect on Charge Trapping Behavior of PP/POE/Silica Nanodielectrics**

Various dielectric nanocomposite materials are studied in the frame of the European Commission funded project GRIDABLE. This project has the aim to develop DC cable extruded insulation and medium and low voltage DC capacitor films exhibiting enhanced performance with respect to presently used materials. The nanocomposites intended for cable applications are polypropylene (PP)/polyolefin elastomer (POE) blends filled with surface modified nano-silica particles. The surface modification is carried out via the state-of-the-art solution method using a polar silane as the modifying agent. Thermally Stimulated Depolarization Current (TSDC) measurements were carried out in order to study the charge trapping behavior of the nanocomposite samples. TSDC results indicate that the addition of the treated nano-silica, for most cases, reduces the density of the deep traps significantly. The effect of the addition of silica nanoparticles - both modified and unmodified - on the crystallinity of the samples was studied using X-ray Diffraction (XRD). This is important as the charge trapping properties of the nanodielectrics can be affected by the degree of crystallinity. While more detailed studies are necessary, these results imply that the depth and the density of the deep trap states is profoundly influenced by the level of the silica modification i.e. the amount of the grafted silane on the silica surface.

#### **General information**

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Electrical Engineering, Research area: Power engineering, Research group: High voltage engineering, University of Twente, VTT Technical Research Centre of Finland

Contributors: Mahtabani, A., Rytöluoto, I., He, X., Saarimäki, E., Lahti, K., Paajanen, M., Anyszka, R., Dierkes, W., Blume, A.

Pages: 129-133

Publication date: 8 Aug 2019

#### **Host publication information**

Title of host publication: Proceedings of the 26th Nordic Insulation Symposium

Place of publication: NTNU, Norway

Publisher: Nordic Insulation Symposium

#### **Publication series**

Name: Proceedings of the Nordic Insulation Symposium

Publisher: Nordic Insulation Symposium

ISSN (Electronic): 2535-3969

Electronic versions:

Solution Modified Fumed Silica and Its Effect on Charge Trapping Behavior of PP Nanodielectrics

DOIs:

10.5324/nordis.v0i26.3292

URLs:

<http://urn.fi/URN:NBN:fi:tuni-201912207050>

#### **Bibliographical note**

EXT="Rytöluoto, Ilkka"

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

### **The Effect of ELF electric fields on Implantable Cardioverter Defibrillators (ICD)**

#### **General information**

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Department of Energy and Process Engineering

Contributors: Gonzalez, J. A., Tarao, H., Korpinen, L.

Number of pages: 3

Pages: 104-106

Publication date: 2012

#### **Host publication information**

Title of host publication: The Bioelectromagnetics Society 34th Annual Meeting, June 17, 2012 - June 22, 2012, Brisbane, Australia  
Publisher: The Bioelectromagnetics Society  
ISBN (Print): 978-0-646-57844-6

#### Publication series

Name: The Bioelectromagnetics Society Annual Meeting  
URLs:  
<http://www.bems2012.com.au/2012/>

#### Bibliographical note

ei ut-numeroa 13.8.2013<br/>Contribution: organisation=epr,FACT1=1<br/>Publisher name: The Bioelectromagnetics Society  
Source: researchoutputwizard  
Source ID: 4099  
Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

### The effects of coating structure and water-holding capacity on the oxygen-scavenging capacity of enzymes embedded in the coating layer

#### General information

Publication status: Published  
MoE publication type: A4 Article in a conference publication  
Organisations: Department of Energy and Process Engineering  
Contributors: Johansson, K., Christophliemk, H., Johansson, C., Jönsson, L. J., Järnström, L.  
Pages: 57-69  
Publication date: 2012

#### Host publication information

Title of host publication: 12th TAPPI Advanced Coating Fundamentals Symposium Proceedings, September 10-12, 2012, Atlanta, USA  
Publisher: TAPPI  
ISBN (Print): 978-1-59510-220-1

#### Publication series

Name: TAPPI Advanced Coating Fundamentals Symposium

#### Bibliographical note

ei ut-numeroa 19.8.2013<br/>Contribution: organisation=epr,FACT1=1<br/>Publisher name: TAPPI  
Source: researchoutputwizard  
Source ID: 4353  
Research output: Chapter in Book/Report/Conference proceeding > Conference contribution > Scientific > peer-review

### Top layer coatability on barrier coatings

#### General information

Publication status: Published  
MoE publication type: A4 Article in a conference publication  
Organisations: Department of Energy and Process Engineering  
Contributors: Bollström, R., Tuominen, M., Määtänen, A., Peltonen, J., Toivakka, M.  
Number of pages: 11  
Pages: 1-11  
Publication date: 2011

#### Host publication information

Title of host publication: TAPPI's PaperCon 2011, May 1-4, 2011, Covington, KY, USA. Paper 360 - Special PaperCon Edition  
Place of publication: Norcross, GA  
Publisher: TAPPI

#### Publication series

Name: TAPPI International Conference Papercon  
Publisher: TAPPI  
URLs:  
<http://www.tappi.org/Downloads/Conference-Papers/2011/2011-PaperCon-Conference/11PAP01.aspx>

**Bibliographical note**

ei ut-numeroa 9.11.2013<br/>Contribution: organisation=epr,pap,FACT1=1

Source: researchoutputwizard

Source ID: 5790

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

**Two-phase PIV/PTV measurement of bubbly flow across pin fins in a micro-channel****General information**

Publication status: Published

MoE publication type: A4 Article in a conference publication

Organisations: Department of Energy and Process Engineering

Contributors: Honkanen, M., Jung, J., Kuo, C. J., Peles, Y., Amitay, M.

Number of pages: 9

Pages: 1-9

Publication date: 2010

**Host publication information**

Title of host publication: 7th International Conference on Multiphase Flow ICMF2010, May 30 - June 4, 2010, Tampa, Florida

URLs:

<http://conferences.dce.ufl.edu/ICMF2010/>

**Bibliographical note**

Contribution: organisation=epr,FACT1=1

Source: researchoutputwizard

Source ID: 8094

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Scientific › peer-review

**The effect of physical adhesion promotion treatments on interfacial adhesion in cellulose-epoxy composite****General information**

Publication status: Published

MoE publication type: D3 Professional conference proceedings

Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Research group: Paper Converting and Packaging

Contributors: Siljander, S., Lehmonen, J., Tanaka, A., Ketoja, J., Heikkilä, P., Lahti, J., Sarlin, E., Vuorinen, J.

Number of pages: 10

Publication date: 2015

**Host publication information**

Title of host publication: Proceedings of the 20th International Conference on Composite Materials

URLs:

<http://iccm20.org/fullpapers/file?f=WM39KAy5r2>

**Bibliographical note**

ISBN- tai ISSN-numeroa kysytty, ei löydy

Research output: Chapter in Book/Report/Conference proceeding › Conference contribution › Professional

**Titanium oxide based nanoparticles by laser ablation in supercritical carbon dioxide****General information**

Publication status: Published

Organisations: Materials Science, Research group: Ceramic materials

Contributors: Levänen, E., Singh, A.

Publication date: Aug 2018

Peer-reviewed: Unknown

Event: Paper presented at The 8th International Conference on Manipulation, Manufacturing and measurement on the Nanoscale, China.

Research output: Other conference contribution › Paper, poster or abstract › Scientific

**Utilization of CO2 in modification of galvanized steel surface**

### General information

Publication status: Published

Organisations: Materials Science, Faculty of Engineering Sciences, Top Analytica Oy, VTT, Valtion teknillinen tutkimuskeskus, SSAB Europe Oy, Tampere Univ Technol, Tampere University of Technology, Dept Mat Sci, VTT Technical Research Centre of Finland

Contributors: Nikkanen, J., Kaleva, A., Saarimaa, V., Honkanen, M., Vuorinen, T., Heinonen, S., Väisänen, P., Markkula, A., Huttunen-Saarivirta, E., Levänen, E.

Publication date: 19 Jun 2018

Peer-reviewed: Unknown

Event: Paper presented at The International Symposium on Inorganic and Environmental Materials 2018, Ghent, Belgium.

Electronic versions:

ISIEM Abstract Nikkanen et al

Research output: Other conference contribution > Paper, poster or abstract > Scientific

### Towards material excellence: Evaluation of Tekes' programmes on materials

#### General information

Publication status: Published

MoE publication type: D4 Published development or research report or study

Organisations: Department of Materials Science, Research group: Plastics and Elastomer Technology, Virebit Oy

Contributors: Timonen, J., Antikainen, M., Das, A., Sarlin, E., Vuorinen, J.

Number of pages: 61

Publication date: 2016

#### Publication information

Publisher: Tekes

ISBN (Print): 978-952-457-621-5

Original language: English

URLs:

<http://www.tekes.fi/tekes/julkaisut1/towards-material-excellence--42016/>

Research output: Book/Report > Commissioned report > Professional

### Anaerobic treatment and resource recovery from methanol rich waste gases and wastewaters

Methanol is an important volatile organic compound (VOC) present in the gaseous and liquid effluents of process industries such as pulp and paper, paint manufacturing and petroleum refineries. An estimated 55,377 tonnes of methanol was emitted to the atmosphere in the year 2017 in the United States alone and at least 65% of the total emission was from the Kraft mills of the pulp and paper industries. The anaerobic biological treatment of methanol-rich gaseous and liquid effluents was tested in two bioreactor configurations, namely a biotrickling filter (BTF) and an upflow anaerobic sludge blanket (UASB) reactor. The volatile fatty acids (VFA) produced in these bioreactors were quantified and a mass balance analysis was carried out. Gas-phase methanol removal along with thiosulfate (~ 1000 mg/L) reduction was carried out for 123 d in an anoxic BTF. A maximum elimination capacity (EC<sub>max</sub>) of 21 g/m<sup>3</sup>.h for methanol and complete removal of thiosulfate was achieved. To examine the gas-phase methanol removal along with selenate reduction, another anoxic BTF was operated for 89 d under step and continuous selenate feeding, wherein the selenate removal efficiency was > 90% and ~ 68%, respectively, during step and continuous selenate feed and a methanol EC<sub>max</sub> of 46 g/m<sup>3</sup>.h was achieved. The anaerobic bioreduction of selenate coupled to methane oxidation was investigated in batch reactors and a BTF inoculated with marine sediment and operated for a period of 348 d. Complete reduction of up to 140 mg/L of step fed selenate was achieved in the BTF. Furthermore, the effect of selenate, sulfate and thiosulfate on methanol utilization for VFA production was individually examined in batch systems. For the study on liquid-phase methanol, acetogenesis of foul condensate (FC) obtained from a chemical pulping industry was tested in three UASB reactors operated at 22, 37 and 55 °C for 51 d. A maximum methanol removal efficiency of 45% in the 55 °C reactor and nearly complete removal of ethanol and acetone in all UASB reactors was achieved. Prior to acetogenesis of the FC, the UASB reactors were operated for a period of 113 d under conditions reported to induce acetogenesis of methanol-rich synthetic wastewater. The recovery of VFA was explored through adsorption studies using anion exchange resins in batch systems. The trends and capacity of adsorption of individual VFA on Amberlite IRA-67 and Dowex optipore L-493 were examined by fitting the experimental data to adsorption isotherm and kinetic models. Subsequently, a sequential batch process was tested to achieve selective separation of acetate from the VFA mixture.

#### General information

Publication status: Published

MoE publication type: G5 Doctoral dissertation (article)

Organisations: Materials Science and Environmental Engineering

Contributors: Eregowda, T.

Number of pages: 211

Publication date: 23 May 2019

### Publication information

Publisher: Tampere University  
Original language: English

### Publication series

Name: Tampere University Dissertations  
URLs:

<http://urn.fi/URN:ISBN:URN:NBN:fi:tuni-201906172041>. Embargo ended: 23/05/20  
Research output: Book/Report > Doctoral thesis > Collection of Articles

### Modeling Fume Particle Dynamics and Deposition with Alkali Metal Chemistry in Kraft Recovery Boilers

The kraft recovery boiler is the largest single unit in the pulp-making process, which makes its reliable operation important. However, the fuel of the recovery boiler, black liquor, contains large quantities of ash-forming elements that pose challenges to the efficient operation of the boiler. A fraction of these elements vaporizes in the recovery boiler and condenses to form submicron-sized particles, called fume. The fume particles may form fouling deposits on the heat transfer surfaces, cause plugging of the flue gas channels, and even expose the surfaces to corrosion. These problems often lead to unscheduled shutdowns of the boiler, which are expensive due to the large size of the modern pulp mills. Significant savings could be achieved if the behavior of the ash-forming elements could be better predicted. The objective of this thesis is to develop a CFD-based (computational fluid dynamics) model for the alkali metal chemistry, fume particles, and fume deposits in the kraft recovery boiler, and to use the model to simulate real recovery boilers. The model combines 3-dimensional CFD, fine particle dynamics, and equilibrium chemistry in a novel way, and solves the fume particle and deposit composition at different locations in the superheater area of the boiler. The model contains certain limitations, such as the steady-state approximation because a compromise has to be made between accuracy and computational cost, which is a significant factor when developing tools for industrial use. The model has been partially validated with measurements in an operating recovery boiler, and the modeling results are in good qualitative agreement with the measurements. Furthermore, the modeling results suggest that deposition through thermophoresis is the main mechanism of fume deposit formation in a recovery boiler, but also that the direct condensation of alkali chloride vapors to heat transfer surfaces can be significant if the black liquor chlorine content is high. According to the model sensitivity analysis, fume deposit growth seems to be a self-limiting process, since an increase in the deposit thickness lowers the rate of deposition by thermophoresis. Another important result is that chlorine enriches in the deposit layers closer to the tube surfaces, which is a result of the high temperature dependence of alkali chloride condensation. The CFD-based model developed here improves understanding of the fume formation mechanisms, shedding light on processes that would be difficult to investigate through experimental methods alone in the corrosive boiler environment. In particular, the model can simulate how certain operational changes, such as increasing boiler load or steam temperatures, affect the alkali metal and fume behavior. In the future, the model can be utilized in the industry to support the engineering of new recovery boilers, and minimize fouling, plugging, and corrosion problems.

### General information

Publication status: Published  
MoE publication type: G5 Doctoral dissertation (article)  
Organisations: Department of Chemistry and Bioengineering, Research group: Power Plant and Combustion Technology  
Contributors: Leppänen, A.  
Number of pages: 63  
Publication date: 9 Jan 2015

### Publication information

Place of publication: Tampere  
Publisher: Tampere University of Technology  
Volume: 1273  
ISBN (Print): 978-952-15-3433-1  
ISBN (Electronic): 978-952-15-3436-2  
Original language: English

### Publication series

Name: Tampere University of Technology. Publication  
Publisher: Tampere University of Technology  
Volume: 1273  
ISSN (Print): 1459-2045  
Electronic versions:  
leppanen\_1273  
URLs:  
<http://urn.fi/URN:ISBN:978-952-15-3436-2>

### Bibliographical note

Awarding institution: Tampereen teknillinen yliopisto - Tampere University of Technology  
Submitter: Submitted by Aino Leppänen (aino.leppanen@tut.fi) on 2014-12-04T11:42:09Z

No. of bitstreams: 1

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