

**Lubricated icephobic coatings prepared by flame spraying with hybrid feedstock injection**

Donadei, V., Koivuluoto, H., Sarlin, E. & Vuoristo, P., 15 Dec 2020, In : Surface and Coatings Technology. 403, 13 p., 126396.

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

**The effect of substrate pre-treatment on durability of rubber-stainless steel adhesion**

Sarlin, E., Honkanen, M., Lindgren, M., Laihonon, P., Juutilainen, M., Vippola, M. & Vuorinen, J., 1 Dec 2020, In : Surfaces and Interfaces. 21, 9 p., 100646.

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

**On the alignment of ZnO nanowires by Langmuir – Blodgett technique for sensing application**

Baratto, C., Golovanova, V., Faglia, G., Hakola, H., Niemi, T., Tkachenko, N., Nazarchurk, B. & Golovanov, V., 30 Oct 2020, In : Applied Surface Science. 528, 146959.

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

**Fusionsense: Emotion classification using feature fusion of multimodal data and deep learning in a brain-inspired spiking neural network**

Tan, C., Ceballos, G., Kasabov, N. & Subramaniam, N. P., 17 Sep 2020, In : Sensors (Switzerland). 20, 18, 27 p., 5328.

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

**Tail-Oxidized Cholesterol Enhances Membrane Permeability for Small Solutes**

Olżyńska, A., Kulig, W., Mikkolainen, H., Czerniak, T., Jurkiewicz, P., Cwiklik, L., Rog, T., Hof, M., Jungwirth, P. & Vattulainen, I., 8 Sep 2020, In : Langmuir. 36, 35, p. 10438-10447 10 p.

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

**Formation of corrosion products on zinc in wet supercritical and subcritical CO<sub>2</sub>: In-situ spectroscopic study**

Kaleva, A., Tassaing, T., Saarimaa, V., Le Bourdon, G., Väisänen, P., Markkulä, A. & Levänen, E., 1 Sep 2020, In : Corrosion Science. 174, 10 p.

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

**The role of symmetry in the aesthetics of residential building façades using cognitive science methods**

Azemati, H., Jam, F., Ghorbani, M., Dehmer, M., Ebrahimpour, R., Ghanbaran, A. & Emmert-Streib, F., 1 Sep 2020, In : Symmetry. 12, 9, 15 p., 1438.

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

**ClothFace: A Batteryless RFID-Based Textile Platform for Handwriting Recognition**

He, H., Chen, X., Mehmood, A., Raivio, L., Huttunen, H., Raunonen, P. & Virkki, J., 28 Aug 2020, In : Sensors (Basel, Switzerland). 20, 17, 12 p., 4878.

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

**The C-I<sup>-</sup>⋯O-N<sup>+</sup> Halogen Bonds with Tetraiodoethylene and Aromatic N-Oxides**

Truong, K. N., Rautiainen, J. M., Rissanen, K. & Puttreddy, R., 5 Aug 2020, In : Crystal Growth and Design. 20, 8, p. 5330-5337 8 p.

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

**Design principles for non-reciprocal photomechanical actuation**

Lahikainen, M., Zeng, H. & Priimagi, A., 7 Jul 2020, In : Soft Matter. 16, 25, p. 5951-5958 8 p.

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

**Nucleation and growth behavior of Er<sup>3+</sup> doped oxyfluorophosphate glasses**

Ojha, N., Szczodra, A., Boetti, N. G., Massera, J. & Petit, L., 7 Jul 2020, In : RSC Advances. 10, 43, p. 25703-25716 14 p.

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

**Selective hydrogen production at Pt(111) investigated by Quantum Monte Carlo methods for metal catalysis**

Sharma, R. O., Rantala, T. T. & Hoggan, P. E., 5 Jun 2020, In : International Journal of Quantum Chemistry. 120, 11, e26198.

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

#### **Additive manufacturing of monolithic supercapacitors with biopolymer separator**

Arvani, M., Keskinen, J., Railanmaa, A., Siljander, S., Björkqvist, T., Tuukkanen, S. & Lupo, D., 1 Jun 2020, In : *Journal of Applied Electrochemistry*. 50, 6, p. 689-697 9 p.

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

#### **Molecular Docking Studies of Royleanone Diterpenoids from *Plectranthus* spp. as P-Glycoprotein Inhibitors**

Isca, V. M. S., Ferreira, R. J., Garcia, C., Monteiro, C. M., Dinic, J., Holmstedt, S., André, V., Pesic, M., Dos Santos, D. J. V. A., Candeias, N. R., Afonso, C. A. M. & Rijo, P., 14 May 2020, In : *ACS MEDICINAL CHEMISTRY LETTERS*. 11, 5, p. 839-845 7 p.

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

#### **Physical Characteristics of Particle Emissions from a Medium Speed Ship Engine Fueled with Natural Gas and Low-Sulfur Liquid Fuels**

Alanen, J., Isotalo, M., Kuittinen, N., Simonen, P., Martikainen, S., Kuuluvainen, H., Honkanen, M., Lehtoranta, K., Nyssönen, S., Vesala, H., Timonen, H., Aurela, M., Keskinen, J. & Rönkkö, T., 5 May 2020, In : *Environmental Science and Technology*. 54, 9, p. 5376-5384 9 p.

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

#### **Rotational Diffusion of Membrane Proteins in Crowded Membranes**

Javanainen, M., Ollila, O. H. S. & Martinez-Seara, H., 16 Apr 2020, In : *Journal of Physical Chemistry B*. 124, 15, p. 2994-3001 8 p.

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

#### **The effect of start-up on energy recovery and compositional changes in brewery wastewater in bioelectrochemical systems**

Haavisto, J. M., Kokko, M. E., Lakaniemi, A. M., Sulonen, M. L. K. & Puhakka, J. A., 1 Apr 2020, In : *BIOELECTROCHEMISTRY*. 132, 8 p., 107402.

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

#### **Host-Guest Interactions of Sodiumsulfonatomethyleneresorcinarene and Quaternary Ammonium Halides: An Experimental-Computational Analysis of the Guest Inclusion Properties**

Twum, K., Rautiainen, J. M., Yu, S., Truong, K. N., Feder, J., Rissanen, K., Puttreddy, R. & Beyeh, N. K., 1 Apr 2020, In : *Crystal Growth and Design*. 20, 4, p. 2367-2376 10 p.

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

#### **Photostable orange-red fluorescent unsymmetrical diketopyrrolopyrrole-BF<sub>2</sub> hybrids**

Young, D. C., Tasiar, M., Laurent, A. D., Dobrzycki, Ł., Cyrański, M. K., Tkachenko, N., Jacquemin, D. & Gryko, D. T., Apr 2020, In : *Journal of Materials Chemistry C*. 8, 23, p. 7708-7717 10 p.

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

#### **Linking volatile and non-volatile compounds to sensory profiles and consumer liking of wild edible Nordic mushrooms**

Aisala, H., Manninen, H., Laaksonen, T., Linderborg, K. M., Myoda, T., Hopia, A. & Sandell, M., 30 Jan 2020, In : *Food Chemistry*. 304, 125403.

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

#### **Sequential Collinear Photofragmentation and Atomic Absorption Spectroscopy for Online Laser Monitoring of Triatomic Metal Species**

Viljanen, J., Kalmankoski, K., Contreras, V., Sarin, J. K., Sorvajärvi, T., Kinnunen, H., Enestam, S. & Toivonen, J., 18 Jan 2020, In : *Sensors (Basel, Switzerland)*. 20, 2, 14 p., 533.

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

#### **Syndecan-4 tunes cell mechanics by activating the kindlin-integrin-RhoA pathway**

Chronopoulos, A., Thorpe, S. D., Cortes, E., Lachowski, D., Rice, A. J., Mykuliak, V. V., Rog, T., Lee, D. A., Hytönen, V. P. & del Río Hernández, A. E., 2020, In : *Nature Materials*. 15 p.

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

### Monitoring Charge Carrier Diffusion across a Perovskite Film with Transient Absorption Spectroscopy

Pasanen, H. P., Vivo, P., Canil, L., Hempel, H., Unold, T., Abate, A. & Tkachenko, N. V., 2020, In : The journal of physical chemistry letters. 11, 2, p. 445-450 6 p.

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

### Effect of tungsten and selenium on C<sub>1</sub> gas bioconversion by an enriched anaerobic sludge and microbial community analysis

Chakraborty, S., Rene, E. R., Lens, P. N. L., Rintala, J., Veiga, M. C. & Kennes, C., 2020, In : Chemosphere. 250, 9 p., 126105.

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

### Compounding and characterization of recycled multilayer plastic films

Jönkkäri, I., Poliakova, V., Mylläri, V., Anderson, R., Andersson, M. & Vuorinen, J., 2020, In : Journal of Applied Polymer Science. 8 p., e49101.

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

### Taste compound – Nanocellulose interaction assessment by fluorescence indicator displacement assay

Manninen, H., Durandin, N., Hopia, A., Vuorimaa-Laukkanen, E. & Laaksonen, T., 2020, In : Food Chemistry. 318, 6 p., 126511.

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

### Hematite Surface Modification toward Efficient Sunlight-Driven Water Splitting Activity: The Role of Gold Nanoparticle Addition

Tofanello, A., Freitas, A. L. M., Carvalho, W. M., Salminen, T., Niemi, T. & Souza, F. L., 2020, In : Journal of Physical Chemistry C.

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

### Influence of powder properties on residual stresses formed in high-pressure liquid fuel HVOF sprayed WC-CoCr coatings

Varis, T., Suhonen, T., Jokipii, M. & Vuoristo, P., 2020, In : Surface and Coatings Technology. 388, 9 p., 125604.

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

### Non-radiative decay and fragmentation in water molecules after 1 a 1-1 4 a 1 excitation and core ionization studied by electron-energy-resolved electron-ion coincidence spectroscopy

Sankari, A., Strähman, C., Sankari, R., Partanen, L., Laksman, J., Kettunen, J. A., Galván, I. F., Lindh, R., Malmqvist, P. Å. & Sorensen, S. L., 2020, In : Journal of Chemical Physics. 152, 7, 7 p., 074302.

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

### Comparison and impact of different fiber debond techniques on fiber reinforced flexible composites

Beter, J., Schrittmesser, B., Maroh, B., Sarlin, E., Fuchs, P. F. & Pinter, G., 2020, In : Polymers. 12, 2, 11 p., 472.

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

### Experimental study on axially loaded square hollow section T-joints under fire conditions

Bączkiewicz, J., Malaska, M., Pajunen, S., Alanen, M. & Heinisuo, M., 2020, In : FIRE SAFETY JOURNAL. 114, 15 p., 102993.

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

### High-resolution analysis of the $\nu_3$ band of radiocarbon methane $^{14}\text{CH}_4$

Larnimaa, S., Halonen, L., Karhu, J., Tomberg, T., Metsälä, M., Genoud, G., Hieta, T., Bell, S. & Vainio, M., 2020, In : Chemical Physics Letters. 750, 5 p., 137488.

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

### Ultrafast Photochemistry of the $[\text{Cr}(\text{NCS})_6]^{3-}$ Complex in Dimethyl Sulfoxide and Dimethylformamide upon Excitation into Ligand-Field Electronic State

Khvorost, T. A., Beliaev, L. Y., Potalueva, E., Laptchenkova, A. V., Selyutin, A. A., Bogachev, N. A., Skripkin, M. Y., Ryazantsev, M. N., Tkachenko, N. & Mereshchenko, A. S., 2020, In : Journal of Physical Chemistry B. 124, 18, p. 3724-3733 10 p.

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

### **Efficient Conversion of Light to Chemical Energy: Directional, Chiral Photoswitches with Very High Quantum Yields**

Moormann, W., Tellkamp, T., Stadler, E., Röhricht, F., Näther, C., Puttreddy, R., Rissanen, K., Gescheidt, G. & Herges, R., 2020, In : *Angewandte Chemie - International Edition*. 59, 35, p. 15081-15086 6 p.

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

### **Modelling of a pressure swing adsorption unit by deep learning and artificial Intelligence tools**

Oliveira, L. M. C., Koivisto, H., Iwakiri, I. G. I., Loureiro, J. M., Ribeiro, A. M. & Nogueira, I. B. R., 2020, In : *Chemical Engineering Science*. 224, 115801.

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

### **Fast Switching of Bright Whiteness in Channeled Hydrogel Networks**

Eklund, A., Zhang, H., Zeng, H., Priimägi, A. & Ikkala, O., 2020, In : *Advanced Functional Materials*. 2000754.

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

### **A concise synthesis of carbasugars isolated from *Streptomyces lincolnensis***

Holmstedt, S. & Candeias, N. R., 2020, In : *Tetrahedron*. 6 p., 131346.

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

### **Bringing a Molecular Plus One: Synergistic Binding Creates Guest-Mediated Three-Component Complexes**

Taimoory, S. M., Twum, K., Dashti, M., Pan, F., Lahtinen, M., Rissanen, K., Puttreddy, R., Trant, J. F. & Beyeh, N. K., 2020, In : *Journal of Organic Chemistry*. 85, 9, p. 5884-5894 11 p.

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

### **A bifacial colour-tunable system via combination of a cholesteric liquid crystal network and hydrogel**

Wani, O. M., Schenning, A. P. H. J. & Priimagi, A., 2020, In : *Journal of Materials Chemistry C*. 8, 30, p. 10191-10196 6 p.

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

### **Modification of Surface States of Hematite-Based Photoanodes by Submonolayer of TiO<sub>2</sub> for Enhanced Solar Water Splitting**

Palmolahti, L., Ali-Löytty, H., Khan, R., Saari, J., Tkachenko, N. V. & Valden, M., 2020, In : *Journal of Physical Chemistry C*. 124, 24, p. 13094-13101 8 p.

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

### **Recovery characteristics of different tube materials in relation to combustion products**

Karjalainen, M., Kontunen, A., Mäkelä, M., Anttalainen, O., Vehkaoja, A., Oksala, N. & Roine, A., 2020, In : *International Journal for Ion Mobility Spectrometry*. 8 p.

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

### **Photo-oxidation of Aromatic Hydrocarbons Produces Low-Volatility Organic Compounds**

Wang, M., Chen, D., Xiao, M., Ye, Q., Stolzenburg, D., Hofbauer, V., Ye, P., Vogel, A. L., Mauldin, R. L., Amorim, A., Baccarini, A., Baumgartner, B., Brilke, S., Dada, L., Dias, A., Duplissy, J., Finkenzeller, H., Garmash, O., He, X. C., Hoyle, C. R., Kim, C., Kvashnin, A., Lehtipalo, K., Fischer, L., Molteni, U., Petäjä, T., Pospisilova, V., Quéléver, L. L. J., Rissanen, M., Simon, M., Tauber, C., Tomé, A., Wagner, A. C., Weitz, L., Volkamer, R., Winkler, P. M., Kirkby, J., Worsnop, D. R., Kulmala, M., Baltensperger, U., Dommen, J., El-Haddad, I. & Donahue, N. M., 2020, In : *Environmental Science and Technology*. 54, 13, p. 7911-7921 11 p.

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

### **Kinetics and modelling of thiosulphate biotransformations by haloalkaliphilic *Thioalkalivibrio versutus***

Hajdu-Rahkama, R., Özkaya, B., Lakaniemi, A. M. & Puhakka, J. A., 2020, In : *Chemical Engineering Journal*. 401, 9 p., 126047.

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

### **Energy dissipation in natural rubber latex films: The effect of stabilizers, leaching and acetone-treatment**

Shakun, A., Sarlin, E. & Vuorinen, J., 2020, In : *Journal of Applied Polymer Science*. 15 p.

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

#### **Conductivity control via minimally invasive anti-Frenkel defects in a functional oxide**

Evans, D. M., Holstad, T. S., Mosberg, A. B., Småbråten, D. R., Vullum, P. E., Dadlani, A. L., Shapovalov, K., Yan, Z., Bourret, E., Gao, D., Akola, J., Torgersen, J., van Helvoort, A. T. J., Selbach, S. M. & Meier, D., 2020, In : *Nature Materials*. 7 p.

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

#### **A modular brain-on-a-chip for modelling epileptic seizures with functionally connected human neuronal networks**

Pelkonen, A., Mzezewa, R., Sukki, L., Rynnänen, T., Kreutzer, J., Hyvärinen, T., Vinogradov, A., Aarnos, L., Lekkala, J., Kallio, P. & Narkilahti, S., 2020, In : *Biosensors and Bioelectronics*. 168, 10 p., 112553.

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

#### **ILC1 drive intestinal epithelial and matrix remodelling**

Jowett, G. M., Norman, M. D. A., Yu, T. T. L., Rosell Arévalo, P., Hoogland, D., Lust, S. T., Read, E., Hamrud, E., Walters, N. J., Niazi, U., Chung, M. W. H., Marciano, D., Omer, O. S., Zabinski, T., Danovi, D., Lord, G. M., Hilborn, J., Evans, N. D., Dreiss, C. A., Bozec, L., Oommen, O. P., Lorenz, C. D., da Silva, R. M. P., Neves, J. F. & Gentleman, E., 2020, In : *Nature Materials*. 22 p.

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

#### **Environmental monitoring with distributed mesh networks: An overview and practical implementation perspective for urban scenario**

Ometov, A., Bezzateev, S., Voloshina, N., Masek, P. & Komarov, M., 2 Dec 2019, In : *Sensors (Switzerland)*. 19, 24, 19 p., 5548.

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

#### **Programmable responsive hydrogels inspired by classical conditioning algorithm**

Zhang, H., Zeng, H., Priimägi, A. & Ikkala, O., 1 Dec 2019, In : *Nature Communications*. 10, 1, 3267.

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

#### **Key drivers of cloud response to surface-active organics**

Lowe, S. J., Partridge, D. G., Davies, J. F., Wilson, K. R., Topping, D. & Riipinen, I., 1 Dec 2019, In : *Nature Communications*. 10, 1, 12 p., 5214.

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

#### **The role of highly oxygenated organic molecules in the Boreal aerosol-cloud-climate system**

Roldin, P., Ehn, M., Kurtén, T., Olenius, T., Rissanen, M. P., Sarnela, N., Elm, J., Rantala, P., Hao, L., Hyttinen, N., Heikkinen, L., Worsnop, D. R., Pichelstorfer, L., Xavier, C., Clusius, P., Öström, E., Petäjä, T., Kulmala, M., Vehkamäki, H., Virtanen, A., Riipinen, I. & Boy, M., 1 Dec 2019, In : *Nature Communications*. 10, 1, 4370.

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

#### **Spectral object recognition in hyperspectral holography with complex-domain denoising**

Shevkunov, I., Katkovnik, V., Claus, D., Pedrini, G., Petrov, N. V. & Egiazarian, K., 26 Nov 2019, In : *Sensors (Switzerland)*. 19, 23, 10 p., 5188.

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

#### **Nanocluster Aerosol Emissions of a 3D Printer**

Poikkimäki, M., Koljonen, V., Leskinen, N., Närhi, M., Kangasniemi, O., Kausiala, O. & Dal Maso, M., 7 Nov 2019, In : *Environmental Science and Technology*. 53, 23, p. 13618–13628 11 p.

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

#### **Molecular Composition and Volatility of Nucleated Particles from $\alpha$ -Pinene Oxidation between $-50\text{ }^{\circ}\text{C}$ and $+25\text{ }^{\circ}\text{C}$**

Ye, Q., Wang, M., Hofbauer, V., Stolzenburg, D., Chen, D., Schervish, M., Vogel, A., Mauldin, R. L., Baalbaki, R., Brilke, S., Dada, L., Dias, A., Duplissy, J., El Haddad, I., Finkenzeller, H., Fischer, L., He, X., Kim, C., Kürten, A., Lamkaddam, H., Lee, C. P., Lehtipalo, K., Leiminger, M., Manninen, H. E., Marten, R., Mentler, B., Partoll, E., Petäjä, T., Rissanen, M., Schobesberger, S., Schuchmann, S., Simon, M., Tham, Y. J., Vazquez-Pufleau, M., Wagner, A. C., Wang, Y., Wu, Y., Xiao, M., Baltensperger, U., Curtius, J., Flagan, R., Kirkby, J., Kulmala, M., Volkamer, R., Winkler, P. M., Worsnop, D. & Donahue, N. M., 5 Nov 2019, In : *Environmental Science and Technology*. 53, 21, p. 12357–12365 9 p.

### **Statistical evaluation of barkhausen noise testing (BNT) for ground samples**

Tomkowski, R., Sorsa, A., Santa-Aho, S., Lundin, P. & Vippola, M., 1 Nov 2019, In : *Sensors (Switzerland)*. 19, 21, 4716.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Controlled Orientations of Neighboring Tetracene Units by Mixed Self-Assembled Monolayers on Gold Nanoclusters for High-Yield and Long-Lived Triplet Excited States through Singlet Fission**

Saegusa, T., Sakai, H., Nagashima, H., Kobori, Y., Tkachenko, N. V. & Hasobe, T., 18 Sep 2019, In : *Journal of the American Chemical Society*. 141, 37, p. 14720-14727 8 p.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Effects of anode materials on electricity production from xylose and treatability of TMP wastewater in an up-flow microbial fuel cell**

Haavisto, J., Dessì, P., Chatterjee, P., Honkanen, M., Noori, M. T., Kokko, M., Lakaniemi, A. M., Lens, P. N. L. & Puhakka, J. A., 15 Sep 2019, In : *Chemical Engineering Journal*. 372, p. 141-150 10 p.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Multiresonant High-Q Plasmonic Metasurfaces**

Reshef, O., Saad-Bin-Alam, M., Huttunen, M. J., Carlow, G., Sullivan, B. T., Ménard, J. M., Dolgaleva, K. & Boyd, R. W., 11 Sep 2019, In : *Nano Letters*. 19, 9, p. 6429-6434 6 p.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Strategies To Diminish the Emissions of Particles and Secondary Aerosol Formation from Diesel Engines**

Karjalainen, P., Rönkkö, T., Simonen, P., Ntziachristos, L., Juuti, P., Timonen, H., Teinilä, K., Saarikoski, S., Saveljeff, H., Lauren, M., Happonen, M., Matilainen, P., Maunula, T., Nuottimäki, J. & Keskinen, J., 3 Sep 2019, In : *Environmental science & technology*. 53, 17, p. 10408-10416 9 p.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Porous polybutylene succinate films enabling adhesion of human embryonic stem cell-derived retinal pigment epithelial cells (hESC-RPE)**

Calejo, M. T., Haapala, A., Skottman, H. & Kellomäki, M., 1 Sep 2019, In : *European Polymer Journal*. 118, p. 78-87 10 p.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Behavior of the DPH fluorescence probe in membranes perturbed by drugs**

Poojari, C., Wilkosz, N., Lira, R. B., Dimova, R., Jurkiewicz, P., Petka, R., Kepczynski, M. & Róg, T., 1 Sep 2019, In : *Chemistry and Physics of Lipids*. 223, 104784.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Influence of ions to modulate hydrazone and oxime reaction kinetics to obtain dynamically cross-linked hyaluronic acid hydrogels**

Wang, S., Nawale, G. N., Oommen, O. P., Hilborn, J. & Varghese, O. P., 21 Aug 2019, In : *Polymer Chemistry*. 10, 31, p. 4322-4327 6 p.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Characterizing the micro-impact fatigue behavior of APS and HVOF-sprayed ceramic coatings**

Kiilakoski, J., Langlade, C., Koivuluoto, H. & Vuoristo, P., 15 Aug 2019, In : *Surface and Coatings Technology*. 371, p. 245-254  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Chlorine induced high-temperature corrosion mechanisms in HVOF and HVOF sprayed Cr<sub>3</sub>C<sub>2</sub>-based hardmetal coatings**

Fantozzi, D., Matikainen, V., Uusitalo, M., Koivuluoto, H. & Vuoristo, P., 14 Aug 2019, In : *Corrosion Science*. 108166.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Bayesian inversion of a forest reflectance model using Sentinel-2 and Landsat 8 satellite images**

Schraik, D., Varvia, P., Korhonen, L. & Rautiainen, M., 1 Aug 2019, In : *JOURNAL OF QUANTITATIVE SPECTROSCOPY AND RADIATIVE TRANSFER*. 233, p. 1-12 12 p.

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

### **Photochemistry of dithiophosphate Ni(S<sub>2</sub>P(i-Bu)<sub>2</sub>)<sub>2</sub> complex in CCl<sub>4</sub>. Transient species and TD-DFT calculations**

Solovyev, A. I., Mikheyliis, A. V., Plyusnin, V. F., Shubin, A. A., Grivin, V. P., Larionov, S. V., Tkachenko, N. V. & Lemmetyinen, H., 1 Aug 2019, In : Journal of Photochemistry and Photobiology A: Chemistry. 381, 111857.

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

### **Erosion wear performance of WC-10Co4Cr and Cr<sub>3</sub>C<sub>2</sub>-25NiCr coatings sprayed with high-velocity thermal spray processes**

Matikainen, V., Rubio Peregrina, S., Ojala, N., Koivuluoto, H., Schubert, J., Houdková & Vuoristo, P., 25 Jul 2019, In : Surface and Coatings Technology. 370, p. 196-212 17 p.

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

### **Observation of Coexistence of Yu-Shiba-Rusinov States and Spin-Flip Excitations**

Kezilebieke, S., Žitko, R., Dvorak, M., Ojanen, T. & Liljeroth, P., 10 Jul 2019, In : Nano Letters. 19, 7, p. 4614-4619 6 p.

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

### **FCC-hh: The Hadron Collider: Future Circular Collider Conceptual Design Report Volume 3**

Abada, A., Abbrescia, M., AbdusSalam, S. S., Abdyukhanov, I., Abelleira Fernandez, J., Abramov, A., Aburaia, M., Acar, A. O., Adzic, P. R., Agrawal, P., Aguilar-Saavedra, J. A., Aguilera-Verdugo, J. J., Aiba, M., Aichinger, I., Aielli, G., Akay, A., Akhundov, A., Aksakal, H., Albacete, J. L., Albergo, S., Alekou, A., Aleksa, M., Aleksan, R., Alemany Fernandez, R. M., Alexahin, Y., Alía, R. G., Alioli, S., Alipour Tehrani, N., Allanach, B. C., Allport, P. P., Altinli, M., Altmannshofer, W., Ambrosio, G., Amorim, D., Amstutz, O., Anderlini, L., Andreazza, A., Andreini, M., Andriatis, A., Andris, C., Andronic, A., Angelucci, M., Antinori, F., Antipov, S. A., Antonelli, M., Antonello, M., Lehtinen, T., Penttinen, J. P., Salmi, T. & Stenvall, A., 1 Jul 2019, In : European Physical Journal: Special Topics. 228, 4, p. 755-1107 353 p.

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

### **Pyrolytic behavior of lignocellulosic-based polysaccharides**

Ghalibaf, M., Doddapaneni, T. R. K. C. & Alén, R., Jul 2019, In : Journal of Thermal Analysis and Calorimetry. 137, 1, p. 121-131

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

### **Crystalline Wax Esters Regulate the Evaporation Resistance of Tear Film Lipid Layers Associated with Dry Eye Syndrome**

Paananen, R. O., Javanainen, M., Holopainen, J. M. & Vattulainen, I., 25 Jun 2019, In : Journal of Physical Chemistry Letters. 10, 14, p. 3893-3898 6 p.

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

### **Water-Responsive and Mechanically Adaptive Natural Rubber Composites by in Situ Modification of Mineral Filler Structures**

Banerjee, S. S., Hait, S., Natarajan, T. S., Wießner, S., Stöckelhuber, K. W., Jehnichen, D., Janke, A., Fischer, D., Heinrich, G., Busfield, J. J. C. & Das, A., 20 Jun 2019, In : Journal of Physical Chemistry B. 123, 24, p. 5168-5175 8 p.

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

### **Epitaxial phases of high Bi content GaSbBi alloys**

Hilksa, J., Koivusalo, E., Puustinen, J., Suomalainen, S. & Guina, M., 15 Jun 2019, In : Journal of Crystal Growth. 516, p. 67-71 5 p.

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

### **Tailoring Second-Harmonic Emission from (111)-GaAs Nanoantennas**

Sautter, J. D., Xu, L., Miroshnichenko, A. E., Lysevych, M., Volkovskaya, I., Smirnova, D. A., Camacho-Morales, R., Zangeneh Kamali, K., Karouta, F., Vora, K., Tan, H. H., Kauranen, M., Staude, I., Jagadish, C., Neshev, D. N. & Rahmani, M., 12 Jun 2019, In : Nano Letters. 19, 6, p. 3905-3911 7 p.

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

### **The Role of Temperature and Lipid Charge on Intake/Uptake of Cationic Gold Nanoparticles into Lipid Bilayers**

Lolicato, F., Joly, L., Martinez-Seara, H., Fragneto, G., Scoppola, E., Baldelli Bombelli, F., Vattulainen, I., Akola, J. & Maccarini, M., 7 Jun 2019, In : Small. 15, 23, 1805046.

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

**Analytical Expressions for Spring Constants of Capillary Bridges and Snap-in Forces of Hydrophobic Surfaces**

Sariola, V., 4 Jun 2019, In : Langmuir. 35, 22, p. 7129-7135 7 p.

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

**Correlation of Surface Morphology and Interfacial Adhesive Behavior between Cellulose Surfaces: Quantitative Measurements in Peak-Force Mode with the Colloidal Probe Technique**

Lai, Y., Zhang, H., Sugano, Y., Xie, H. & Kallio, P., 4 Jun 2019, In : Langmuir. 35, 22, p. 7312-7321 10 p.

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

**Methods for simultaneous robot-world-hand-eye calibration: A comparative study**

Ali, I., Suominen, O., Gotchev, A. & Morales, E. R., 2 Jun 2019, In : Sensors (Switzerland). 19, 12, 2837.

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

**Bioimpedance Sensor Array for Long-Term Monitoring of Wound Healing from Beneath the Primary Dressings and Controlled Formation of H<sub>2</sub>O<sub>2</sub> Using Low-Intensity Direct Current**

Kekonen, A., Bergelin, M., Johansson, M., Kumar Joon, N., Bobacka, J. & Viik, J., 31 May 2019, In : Sensors. 19, 11

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

**Reaction between Peroxy and Alkoxy Radicals Can Form Stable Adducts**

Iyer, S., Rissanen, M. P. & Kurtén, T., 2 May 2019, In : Journal of Physical Chemistry Letters. 10, 9, p. 2051-2057 7 p.

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

**Energy-dependent diffusion in a soft periodic Lorentz gas**

Gil-Gallegos, S., Klages, R., Solanpää, J. & Räsänen, E., 1 May 2019, In : European Physical Journal: Special Topics. 228, 1, p. 143-160 18 p.

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

**Moiré superlattices and 2D electronic properties of graphite/MoS<sub>2</sub> heterostructures**

Trainer, D. J., Putilov, A. V., Wang, B., Lane, C., Saari, T., Chang, T. R., Jeng, H. T., Lin, H., Xi, X., Nieminen, J., Bansil, A. & Iavarone, M., May 2019, In : Journal of Physics and Chemistry of Solids. 128, p. 325-330

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

**Spin filtering in silicene by edges and chemically or electrically induced interfaces**

Saari, T. & Nieminen, J., May 2019, In : Journal of Physics and Chemistry of Solids. 128, p. 316-324

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

**Mass balance control of crushing circuits**

Itävuo, P., Hulthén, E., Yahyaei, M. & Viikko, M., May 2019, In : Minerals Engineering. 135, p. 37-47 11 p.

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

**Complex Behavior of Phosphatidylcholine-Phosphatidic Acid Bilayers and Monolayers: Effect of Acyl Chain Unsaturation**

Kulig, W., Korolainen, H., Zatorska, M., Kwolek, U., Wydro, P., Kepczynski, M. & Róg, T., 30 Apr 2019, In : Langmuir. 35, 17, p. 5944-5956 13 p.

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

**Analysis of GaAsBi growth regimes in high resolution with respect to As/Ga ratio using stationary MBE growth**

Puustinen, J., Hilska, J. & Guina, M., 1 Apr 2019, In : Journal of Crystal Growth. 511, p. 33-41 9 p.

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

**Hydrolysis and drug release from poly(ethylene glycol)-modified lactone polymers with open porosity**

Asikainen, S., Paakinaho, K., Kyhkynen, A. K., Hannula, M., Malin, M., Ahola, N., Kellomäki, M. & Seppälä, J., 1 Apr 2019, In : European Polymer Journal. 113, p. 165-175 11 p.

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



**Positioning information privacy in intelligent transportation systems: An overview and future perspective**

Ometov, A., Bezzateev, S., Davydov, V., Shchesniak, A., Masek, P., Lohan, E. S. & Koucheryavy, Y., 1 Apr 2019, In : Sensors. 19, 7, 1603.

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

**Alpha radiation-induced luminescence by am-241 in aqueous nitric acid solution**

Kerst, T., Malmbeck, R., Ial Banik, N. L. & Toivonen, J., 1 Apr 2019, In : Sensors (Switzerland). 19, 7, 1602.

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

**The Devil Is in the Details: What Do We Really Track in Single-Particle Tracking Experiments of Diffusion in Biological Membranes?**

Gurtovenko, A. A., Javanainen, M., Lolicato, F. & Vattulainen, I., 7 Mar 2019, In : Journal of Physical Chemistry Letters. 10, 5, p. 1005-1011 7 p.

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

**Kinetics and thermochemistry of the reaction of 3-methylpropargyl radical with molecular oxygen**

Pekkanen, T. T., Timonen, R. S., Lendvay, G., Rissanen, M. P. & Eskola, A. J., 1 Jan 2019, In : PROCEEDINGS OF THE COMBUSTION INSTITUTE. 37, 1, p. 299-306 8 p.

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

**A Pentacene-based Nanotube Displaying Enriched Electrochemical and Photochemical Activities**

Kuroda, K., Yazaki, K., Tanaka, Y., Akita, M., Sakai, H., Hasobe, T., Tkachenko, N. V. & Yoshizawa, M., Jan 2019, In : Angewandte Chemie - International Edition. 58, 4, p. 1115-1119

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

**Charge carrier dynamics in tantalum oxide overlayers and tantalum doped hematite photoanodes**

Ruoko, T-P., Hiltunen, A., Iivonen, T., Ulkuniemi, R., Lahtonen, K., Ali-Löyty, H., Mizohata, K., Valden, M., Leskelä, M. & Tkachenko, N. V., Jan 2019, In : Journal of Materials Chemistry A. 7, 7, p. 3206-3215 10 p.

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

**O<sub>2</sub>-requiring molecular reporters of gene expression for anaerobic microorganisms**

Güglielmetti, S., Santala, V., Mangayil, R., Ciranna, A. & Karp, M. T., 2019, In : Biosensors and Bioelectronics. 123, p. 1-6 6 p.

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

**An automated algorithm for reliable equation of state fitting of magnetic systems**

Levämäki, H., Tian, L-Y., Vitos, L. & Ropo, M., 2019, In : Computational Materials Science. 156, p. 121-128 8 p.

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

**Low-dimensional formamidinium lead perovskite architectures via controllable solvent intercalation**

Shin, M., Kim, J., Jung, Y. K., Ruoko, T-P., Priimagi, A., Walsh, A. & Shin, B., 2019, In : Journal of Materials Chemistry C. 7, 13, p. 3945-3951 7 p.

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

**Tuning of nonlinear absorption in highly luminescent CdSe based quantum dots with core-shell and core/multi-shell architectures**

Bhagyaraj, S., Perumbilavil, S., Udayabashkar, R., Mangalaraja, R. V., Thomas, S., Kalarikkal, N. & Oluwafemi, O. S., 2019, In : Physical Chemistry Chemical Physics. 21, 21, p. 11424-11434 11 p.

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

**Multiphoton Excitation of CsPbBr<sub>3</sub> Perovskite Quantum Dots (PQDs): How Many Electrons Can One PQD Donate to Multiple Molecular Acceptors?**

Mandal, S. & Tkachenko, N. V., 2019, In : Journal of Physical Chemistry Letters. p. 2775-2781 7 p.

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

**Spodumene tailings for porcelain and structural materials: Effect of temperature (1050–1200°C) on the sintering and properties**

Lemougna, P. N., Yliniemi, J., Ismailov, A., Levänen, E., Tanskanen, P., Kinnunen, P., Roning, J. & Illikainen, M., 2019, (Accepted/In press) In : Minerals Engineering. 105843.

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

**Volatile fatty acid adsorption on anion exchange resins: kinetics and selective recovery of acetic acid**

Eregowda, T., Rene, E. R., Rintala, J. & Lens, P. N. L., 2019, In : Separation Science and Technology (Philadelphia).

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

**Possible strategy to use differential mobility spectrometry in real time applications**

Anttalainen, O., Puton, J., Kontunen, A., Karjalainen, M., Kumpulainen, P., Oksala, N., Safaei, Z. & Roine, A., 2019, In : International Journal for Ion Mobility Spectrometry.

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

**Synthesis of 6,12-disubstituted methanodibenzo[b,f][1,5]dioxocins: Pyrrolidine catalyzed self-condensation of 2'-Hydroxyacetophenones**

Assoah, B., Riihonen, V., Vale, J. R., Valkonen, A. & Candeias, N. R., 2019, In : Molecules. 24, 13, 2405.

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

**Metabolic profiling of water-soluble compounds from the extracts of dark septate endophytic fungi (DSE) isolated from Scots pine (*Pinus sylvestris* L.) seedlings using UPLC–orbitrap–MS**

Tienaho, J., Karonen, M., Muilu-Mäkelä, R., Wähälä, K., Denegri, E. L., Franzén, R., Karp, M., Santala, V. & Sarjala, T., 2019, In : Molecules. 24, 12, 2330.

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

**Exclusive occurrence of photoinduced energy transfer and switching of its direction by rectangular  $\pi$ -extension of nanographenes**

Umeyama, T., Hanaoka, T., Yamada, H., Namura, Y., Mizuno, S., Ohara, T., Baek, J., Park, J., Takano, Y., Stranius, K., Tkachenko, N. V. & Imahori, H., 2019, In : Chemical Science. 10, 27, p. 6642-6650 9 p.

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

**The maximum Hosoya index of unicyclic graphs with diameter at most four**

Liu, W., Ban, J., Feng, L., Cheng, T., Emmert-Streib, F. & Dehmer, M., 2019, In : Symmetry. 11, 8, 1034.

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

**The Hosoya entropy of graphs revisited**

Ghorbani, M., Dehmer, M., Mowshowitz, A., Tao, J. & Emmert-Streib, F., 2019, In : Symmetry. 11, 8, 1013.

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

**Temperature scanning stress relaxation behavior of water responsive and mechanically adaptive elastomer nanocomposites**

Banerjee, S. S., Natarajan, T. S., Subramani B., E., Wießner, S., Janke, A., Heinrich, G. & Das, A., 2019, In : Journal of Applied Polymer Science. 48344.

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

**Large-scale efficient water harvesting using bioinspired micro-patterned copper oxide nanoneedle surfaces and guided droplet transport**

Sharma, V., Yiannacou, K., Karjalainen, M., Lahtonen, K., Valden, M. & Sariola, V., 2019, In : Nanoscale Advances. 1, 10, p. 4025-4040 16 p.

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

**Synergistic Computational-Experimental Discovery of Highly Selective PtCu Nanocluster Catalysts for Acetylene Semihydrogenation**

Ayodele, O. B., Cai, R., Wang, J., Ziouani, Y., Liang, Z., Spadaro, M. C., Kovnir, K., Arbiol, J., Akola, J., Palmer, R. E. & Kolen'ko, Y. V., 2019, In : ACS CATALYSIS. p. 451-457 7 p.

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

#### **How well can we predict cluster fragmentation inside a mass spectrometer?**

Passananti, M., Zapadinsky, E., Zanca, T., Kangasluoma, J., Myllys, N., Rissanen, M. P., Kurtén, T., Ehn, M., Attoui, M. & Vehkamäki, H., 2019, In : *Chemical Communications*. 55, 42, p. 5946-5949 4 p.

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

#### **Reversible photodoping of TiO<sub>2</sub> nanoparticles**

Joost, U., Sutka, A., Oja, M., Smits, K., Doebelin, N., Loot, A., Järvekülg, M., Hirsimäki, M., Valden, M. & Nommiste, E., 26 Dec 2018, In : *Chemistry of Materials*. 30, 24, p. 8968-8974

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

#### **Less Is More: Enhancement of Second-Harmonic Generation from Metasurfaces by Reduced Nanoparticle Density**

Czaplicki, R., Kiviniemi, A., Huttunen, M. J., Zang, X., Stolt, T., Vartiainen, I., Butet, J., Kuittinen, M., Martin, O. J. F. & Kauranen, M., 12 Dec 2018, In : *Nano Letters*. 18, 12, p. 7709-7714 6 p.

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

#### **Experimental moment resistance of rectangular hollow section T joints**

Garifullin, M., 5 Dec 2018, In : *MATEC Web of Conferences*. 245, 08003.

Research output: Contribution to journal › Conference article › Scientific › peer-review

#### **Structural basis of actin monomer re-charging by cyclase-Associated protein**

Kotila, T., Kogan, K., Enkavi, G., Guo, S., Vattulainen, I., Goode, B. L. & Lappalainen, P., 1 Dec 2018, In : *Nature Communications*. 9, 1, 1892.

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

#### **Beaming random lasers with soliton control**

Perumbilavil, S., Piccardi, A., Barboza, R., Buchnev, O., Kauranen, M., Strangi, G. & Assanto, G., 1 Dec 2018, In : *Nature Communications*. 9, 1, 7 p., 3863.

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

#### **Machine learning plastic deformation of crystals**

Salmenjoki, H., Alava, M. J. & Laurson, L., 1 Dec 2018, In : *Nature Communications*. 9, 1, 5307.

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

#### **Bi-directional cell-pericellular matrix interactions direct stem cell fate**

Ferreira, S. A., Motwani, M. S., Faull, P. A., Seymour, A. J., Yu, T. T. L., Enayati, M., Taheem, D. K., Salzlechner, C., Haghghi, T., Kania, E. M., Oommen, O. P., Ahmed, T., Loaiza, S., Parzych, K., Dazzi, F., Varghese, O. P., Festy, F., Grigoriadis, A. E., Auner, H. W., Snijders, A. P., Bozec, L. & Gentleman, E., Dec 2018, In : *Nature Communications*. 9, 1, 12 p., 4049.

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

#### **Aminobenzylated 4-Nitrophenols as Antibacterial Agents Obtained from 5-Nitrosalicylaldehyde through a Pétasis Borono-Mannich Reaction**

Rimpiläinen, T., Andrade, J., Nunes, A., Ntungwe, E., Fernandes, A. S., Vale, J. R., Rodrigues, J., Gomes, J. P., Rijo, P. & Candeias, N. R., 29 Nov 2018, In : *ACS Omega*. 3, 11, p. 16191-16202 12 p.

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

#### **Machine learning analysis of extreme events in optical fibre modulation instability**

Närhi, M., Salmela, L., Toivonen, J., Billet, C., Dudley, J. M. & Genty, G., 22 Nov 2018, In : *Nature Communications*. 9, 1, 1 p.

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

#### **High Nitrogen Removal in a Constructed Wetland Receiving Treated Wastewater in a Cold Climate**

Uusheimo, S., Huotari, J., Tulonen, T., Aalto, S. L., Rissanen, A. J. & Arvola, L., 20 Nov 2018, In : *Environmental science & technology*. 52, 22, p. 13343-13350 8 p.

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

**High-Yield Generation of Triplet Excited States by an Efficient Sequential Photoinduced Process from Energy Transfer to Singlet Fission in Pentacene-Modified CdSe/ZnS Quantum Dots**

Sakai, H., Inaya, R., Tkachenko, N. V. & Hasobe, T., 16 Nov 2018, In : Chemistry - A European Journal. 24, 64, p. 17062-17071 10 p.

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

**M2M Communication Assessment in Energy-Harvesting and Wake-Up Radio Assisted Scenarios Using Practical Components**

Rinne, J., Keskinen, J., Berger, P. R., Lupo, D. & Valkama, M., 16 Nov 2018, In : Sensors (Basel, Switzerland). 18, 11

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

**Molecular-Scale Ligand Effects in Small Gold-Thiolate Nanoclusters**

Chevrier, D. M., Raich, L., Rovira, C., Das, A., Luo, Z., Yao, Q., Chatt, A., Xie, J., Jin, R., Akola, J. & Zhang, P., 14 Nov 2018, In : Journal of the American Chemical Society. 140, 45, p. 15430-15436 7 p.

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

**Biological treatment of selenium-laden wastewater containing nitrate and sulfate in an upflow anaerobic sludge bed reactor at pH 5.0**

Tan, L. C., Nancharaiyah, Y. V., Lu, S., van Hullebusch, E. D., Gerlach, R. & Lens, P. N. L., 1 Nov 2018, In : Chemosphere. 211, p. 684-693 10 p.

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

**Tribocorrosion behaviour of aluminium bronze in 3.5 wt.% NaCl solution**

Huttunen-Saarivirta, E., Isotahdon, E., Metsäjoki, J., Salminen, T., Carpén, L. & Ronkainen, H., 1 Nov 2018, In : Corrosion Science. 144, p. 207-223 17 p.

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

**Computation of Dynamic Polarizabilities and van der Waals Coefficients from Path-Integral Monte Carlo**

Tiihonen, J., Kylänpää, I. & Rantala, T. T., 2 Oct 2018, In : Journal of Chemical Theory and Computation. 14, p. 5750-5763 14 p.

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

**Quantification of bio-anode capacitance in bioelectrochemical systems using Electrochemical Impedance Spectroscopy**

Heijne, A. T., Liu, D., Sulonen, M., Sleutels, T. & Fabregat-Santiago, F., 1 Oct 2018, In : Journal of Power Sources. 400, p. 533-538 6 p.

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

**Mechanical, thermal, and burning properties of viscose fabric composites: Influence of epoxy resin modification**

Rajan, R., Rainosalu, E., Ramamoorthy, S. K., Thomas, S. P., Zavašnik, J., Vuorinen, J. & Skrifvars, M., 20 Sep 2018, In : Journal of Applied Polymer Science. 135, 36, 46673.

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

**Electro-concentration for chemical-free nitrogen capture as solid ammonium bicarbonate**

Jermakka, J., Thompson Brewster, E., Ledezma, P. & Freguia, S., 12 Sep 2018, In : Separation and Purification Technology. 203, p. 48-55 8 p.

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

**A compact olfactometer for IMS measurements and testing human perception**

Nieminen, V., Karjalainen, M., Salminen, K., Rantala, J., Kontunen, A., Isokoski, P., Müller, P., Kallio, P., Surakka, V. & Leikkala, J., Sep 2018, In : International Journal for Ion Mobility Spectrometry. 21, 3, p. 71-80 10 p.

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

**Effects of pyrolysis temperature on the hydrologically relevant porosity of willow biochar**

Hyväluoma, J., Hannula, M., Arstila, K., Wang, H., Kulju, S. & Rasa, K., Sep 2018, In : Journal of Analytical and Applied Pyrolysis. 134

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

#### **Photoinduced Energy Transfer in ZnCdSeS Quantum Dot-Phthalocyanines Hybrids**

Mandal, S., Garcia Iglesias, M., Ince, M., Torres, T. & Tkachenko, N. V., 31 Aug 2018, In : ACS Omega. 3, 8, p. 10048-10057 10 p.

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

#### **Selenate removal in biofilm systems: Effect of nitrate and sulfate on selenium removal efficiency, biofilm structure and microbial community**

Tan, L. C., Espinosa-Ortiz, E. J., Nancharaiyah, Y. V., van Hullebusch, E. D., Gerlach, R. & Lens, P. N., Aug 2018, In : Journal of Chemical Technology and Biotechnology. 93, 8, p. 2380-2389

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

#### **Design aspects of all atomic layer deposited TiO<sub>2</sub>-Fe<sub>2</sub>O<sub>3</sub> scaffold-absorber photoanodes for water splitting**

Hiltunen, A., Ruoko, T.-P., Iivonen, T., Lahtonen, K., Ali-Löytty, H., Sarlin, E., Valden, M., Leskelä, M. & Tkachenko, N., 31 Jul 2018, In : Sustainable Energy & Fuels. 2, 9, p. 2124-2130

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

#### **High Bending-Mode Sensitivity of Printed Piezoelectric Poly(vinylidene fluoride- co-trifluoroethylene) Sensors**

Rajala, S., Schouten, M., Krijnen, G. & Tuukkanen, S., 23 Jul 2018, In : ACS Omega. 3, 7, p. 8067-8073 7 p.

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

#### **Pectin and Mucin Enhance the Bioadhesion of Drug Loaded Nanofibrillated Cellulose Films**

Laurén, P., Paukkonen, H., Lipiäinen, T., Dong, Y., Oksanen, T., Rääkkönen, H., Ehlers, H., Laaksonen, P., Yliperttula, M. & Laaksonen, T., 1 Jul 2018, In : Pharmaceutical Research. 35, 7, 145.

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

#### **Effect of surfactant type and sonication energy on the electrical conductivity properties of nanocellulose-CNT nanocomposite films**

Siljander, S., Keinänen, P., Rätty, A., Ramakrishnan, K. R., Tuukkanen, S., Kunnari, V., Harlin, A., Vuorinen, J. & Kanerva, M., 20 Jun 2018, In : International Journal of Molecular Sciences. 19, 6, 1819.

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

#### **Multifunctional nitrogen sulfur co-doped reduced graphene oxide – Ag nano hybrids (sphere, cube and wire) for nonlinear optical and SERS applications**

Nair, A. K., Bhavitha, K. B., Perumbilavil, S., Sankar, P., Rouxel, D., Kala, M. S., Thomas, S. & Kalarikkal, N., 1 Jun 2018, In : Carbon. 132, p. 380-393 14 p.

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

#### **Photo-antimicrobial efficacy of zinc complexes of porphyrin and phthalocyanine activated by inexpensive consumer LED lamp**

George, L., Hiltunen, A., Santala, V. & Efimov, A., 1 Jun 2018, In : Journal of Inorganic Biochemistry. 183, p. 94-100 7 p.

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

#### **Acquiring respiration rate from photoplethysmographic signal by recursive bayesian tracking of intrinsic modes in time-frequency spectra**

Pirhonen, M., Peltokangas, M. & Vehkaoja, A., 1 Jun 2018, In : Sensors. 18, 6, 1693.

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

#### **Evaluation of dry electrodes in canine heart rate monitoring**

Virtanen, J., Somppi, S., Törnqvist, H., Jeyhani, V., Fiedler, P., Gizatdinova, Y., Majaranta, P., Väättäjä, H., Cardó, A. V., Lekkala, J., Tuukkanen, S., Surakka, V., Vainio, O. & Vehkaoja, A., 1 Jun 2018, In : Sensors. 18, 6, 1757.

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

#### **Effect of Co-Adsorbate and Hole Transporting Layer on the Photoinduced Charge Separation at the TiO<sub>2</sub>-Phthalocyanine Interface**

Virkki, K., Tervola, E., Medel, M., Torres, T. & Tkachenko, N. V., 31 May 2018, In : ACS Omega. 3, 5, p. 4947-4958 12 p.  
Research output: Contribution to journal > Article > Scientific > peer-review

**A Ceramide-Regulated Element in the Late Endosomal Protein LAPT4B Controls Amino Acid Transporter Interaction**  
Zhou, K., Dichlberger, A., Martinez-Seara, H., Nyholm, T. K. M., Li, S., Kim, Y. A., Vattulainen, I., Ikonen, E. & Blom, T., 23 May 2018, In : ACS Central Science. 4, 5, p. 548-558 11 p.

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

**Wet etching of dilute nitride GaInNAs, GaInNAsSb, and GaNAsSb alloys lattice-matched to GaAs**

Raappana, M., Polojärvi, V., Aho, A., Mäkelä, J., Aho, T., Tukiainen, A., Laukkanen, P. & Guina, M., 15 May 2018, In : Corrosion Science. 136, p. 268-274 7 p.

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

**Free amino acids and 5'-nucleotides in Finnish forest mushrooms**

Manninen, H., Rotola-Pukkila, M., Aisala, H., Hopia, A. & Laaksonen, T., May 2018, In : Food Chemistry. 247, p. 23-28 6 p.

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

**Characteristics of nFOG, an aerosol-based wet thin film coating technique**

Harra, J., Tuominen, M., Juuti, P., Rissler, J., Koivuluoto, H., Haapanen, J., Niemelä-Anttonen, H., Stenroos, C., Teisala, H., Lahti, J., Kuusipalo, J., Vuoristo, P. & Mäkelä, J. M., May 2018, In : Journal of Coatings Technology Research. 15, 3, p. 623-632 10 p.

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

**Accurate Binding of Sodium and Calcium to a POPC Bilayer by Effective Inclusion of Electronic Polarization**

Melcr, J., Martinez-Seara, H., Nencini, R., Kolafa, J., Jungwirth, P. & Ollila, O. H. S., 26 Apr 2018, In : Journal of Physical Chemistry B. 122, 16, p. 4546-4557 12 p.

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**

Khan, M., Koivisto, J., Hukka, T., Hokka, M. & Kellomäki, M., 11 Apr 2018, In : ACS Applied Materials & Interfaces. 10, 14, p. 11950-11960

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

**Membrane bound COMT isoform is an interfacial enzyme: General mechanism and new drug design paradigm**

Magarkar, A., Parkkila, P., Viitala, T., Lajunen, T., Mobarak, E., Licari, G., Cramariuc, O., Vauthey, E., Róg, T. & Bunker, A., 11 Apr 2018, In : Chemical Communications. 54, 28, p. 3440-3443 4 p.

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

**Properties of HVOF-sprayed Stellite-6 coatings**

Sassatelli, P., Bolelli, G., Lassinantti Gualtieri, M., Heinonen, E., Honkanen, M., Lusvarghi, L., Manfredini, T., Rigon, R. & Vippola, M., 25 Mar 2018, In : Surface and Coatings Technology. 338, p. 45-62 18 p.

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

**Thermal Isomerization of Hydroxyazobenzenes as a Platform for Vapor Sensing**

Poutanen, M., Ahmed, Z., Rautkari, L., Ikkala, O. & Priimägi, A., 20 Mar 2018, In : ACS Macro Letters. 7, 3, p. 381-386 6 p.

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

**Improving the high temperature abrasion resistance of thermally sprayed Cr<sub>3</sub>C<sub>2</sub>-NiCr coatings by WC addition**

Janka, L., Berger, L. M., Norpoth, J., Trache, R., Thiele, S., Tomastik, C., Mätikäinen, V. & Vuoristo, P., 15 Mar 2018, In : Surface and Coatings Technology. 337, p. 296-305 10 p.

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

**Soft hydrazone crosslinked hyaluronan- and alginate-based hydrogels as 3D supportive matrices for human pluripotent stem cell-derived neuronal cells**

Karvinen, J., Joki, T., Ylä-Outinen, L., Koivisto, J. T., Narkilahti, S. & Kellomäki, M., 1 Mar 2018, In : *Reactive and Functional Polymers*. 124, p. 29-39 11 p.

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

**Improved Stability of Atomic Layer Deposited Amorphous TiO<sub>2</sub> Photoelectrode Coatings by Thermally Induced Oxygen Defects**

Hannula, M., Ali-Löyty, H., Lahtonen, K., Sarlin, E., Saari, J. & Valden, M., 27 Feb 2018, In : *Chemistry of Materials*. 30, 4, p. 1199-1208 10 p.

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

**An activity recognition framework deploying the random forest classifier and a single optical heart rate monitoring and triaxial accelerometer wrist-band**

Mehrang, S., Pietilä, J. & Korhonen, I., 22 Feb 2018, In : *Sensors*. 18, 2, 613.

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

**UV-Blocking Synthetic Biopolymer from Biomass-Based Bifuran Diester and Ethylene Glycol**

Kainulainen, T. P., Sirviö, J. A., Sethi, J., Hukka, T. I. & Heiskanen, J. P., 21 Feb 2018, In : *Macromolecules*. 51, 5, p. 1822-1829 8 p.

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

**Pot-economy autooxidative condensation of 2-Aryl-2-lithio-1,3-dithianes**

Vale, J. R., Rimpiläinen, T., Sievänen, E., Rissanen, K., Afonso, C. A. M. & Candeias, N. R., 16 Feb 2018, In : *Journal of Organic Chemistry*. 83, 4, p. 1948-1958 11 p.

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

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

Vaikuntam, S. R., Stöckelhuber, K. W., Subramani Bhagavatheswaran, E., Wießner, S., Scheler, U., Saalwächter, K., Formanek, P., Heinrich, G. & Das, A., 15 Feb 2018, In : *Journal of Physical Chemistry B*. 122, 6, p. 2010-2022 13 p.

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

**MetriIntSimil-an accurate and robust metric for comparison of similarity in intelligence of any number of cooperative multiagent systems**

Iantovics, L. B., Dehmer, M. & Emmert-Streib, F., 1 Feb 2018, In : *Symmetry*. 10, 2, 48.

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

**Controlled Growth of Supported ZnO Inverted Nanopyramids with Downward Pointing Tips**

Barreca, D., Carraro, G., Maccato, C., Altantzis, T., Kaunisto, K. & Gasparotto, A., Feb 2018, In : *Crystal Growth and Design*. 18, 4, p. 2579-2587 9 p.

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

**Temperature scanning stress relaxation of an autonomous self-healing elastomer containing non-covalent reversible network junctions**

Das, A., Sallat, A., Böhme, F., Sarlin, E., Vuorinen, J., Vennemann, N., Heinrich, G. & Stöckelhuber, K. W., 19 Jan 2018, In : *Polymers*. 10, 1, 94.

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

**Concentration-dependent photophysical switching in mixed self-assembled monolayers of pentacene and perylene diimide on gold nanoclusters**

Kato, D., Sakai, H., Araki, Y., Wada, T., Tkachenko, N. V. & Hasobe, T., 1 Jan 2018, In : *Physical Chemistry Chemical Physics*. 20, 13, p. 8695-8706 12 p.

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

**Upconversion from fluorophosphate glasses prepared with NaYF<sub>4</sub>:Er<sup>3+</sup>, Yb<sup>3+</sup> nanocrystals**

Ojha, N., Tuomisto, M., Lastusaari, M. & Petit, L., 1 Jan 2018, In : *RSC Advances*. 8, 34, p. 19226-19236 11 p.

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

**Ortho-Fluorination of azophenols increases the mesophase stability of photoresponsive hydrogen-bonded liquid crystals**

Saccone, M., Kuntze, K., Ahmed, Z., Siiskonen, A., Giese, M. & Priimagi, A., 1 Jan 2018, In : Journal of Materials Chemistry C. 6, 37, p. 9958-9963 6 p.

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

**Improved electromechanical response in acrylic rubber by different carbon-based fillers**

Shakun, A., Poikelispää, M., Das, A. & Vuorinen, J., 2018, In : Polymer Engineering and Science. 58, 3, p. 395-404

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

**Modification of epoxy resin by silane-coupling agent to improve tensile properties of viscose fabric composites**

Rajan, R., Rainosalu, E., Thomas, S. P., Ramamoorthy, S. K., Zavašnik, J., Vuorinen, J. & Skrifvars, M., 2018, In : Polymer Bulletin. 75, 1, p. 167-195 29 p.

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

**Adsorption of furfural from torrefaction condensate using torrefied biomass**

Doddapaneni, T. R. K. C., Jain, R., Praveenkumar, R., Rintala, J., Romar, H. & Konttinen, J., 2018, In : Chemical Engineering Journal. 334, p. 558-568 11 p.

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

**Regeneration of sulfur-poisoned Pd-based catalyst for natural gas oxidation**

Honkanen, M., Wang, J., Kärkkäinen, M., Huuhtanen, M., Jiang, H., Kallinen, K., Keiski, R. L., Akola, J. & Vippola, M., 2018, In : Journal of Catalysis. 358, p. 253-265 13 p.

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

**Composition and role of the attached and planktonic microbial communities in mesophilic and thermophilic xylose-fed microbial fuel cells**

Dessi, P., Porca, E., Haavisto, J., Lakaniemi, A-M., Collins, G. & Lens, P. N. L., 2018, In : RSC Advances. 8, 6, p. 3069-3080 12 p.

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

**Decomposition of persistent luminescent microparticles in corrosive phosphate glass melt**

Ojha, N., Nguyen, H., Laihinne, T., Salminen, T., Lastusaari, M. & Petit, L., 2018, In : Corrosion Science. 135, p. 207-214

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

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

Saarimaa, V., Kaleva, A., Paunikallio, T., Nikkanen, J-P., Heinonen, S., Levänen, E., Väisänen, P. & Markkula, A., 2018, In : Surface and Interface Analysis. 50, 5, p. 564-570

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

**Gloriosa superba Mediated Synthesis of Platinum and Palladium Nanoparticles for Induction of Apoptosis in Breast Cancer**

Rokade, S. S., Joshi, K. A., Mahajan, K., Patil, S., Tomar, G., Dubal, D. S., Parihar, V. S., Kitture, R., Bellare, J. R. & Ghosh, S., 2018, In : Bioinorganic Chemistry and Applications. 2018, 4924186.

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

**A Bioscreening Technique for Ultraviolet Irradiation Protective Natural Substances**

Tienaho, J., Poikulainen, E., Sarjala, T., Muilu-Mäkelä, R., Santala, V. & Karp, M., 2018, In : Photochemistry and Photobiology. 94, 6, p. 1273-1280

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

**Detection and characterization at nM concentration of oligomers formed by hIAPP, A $\beta$ (1-40) and their equimolar mixture using SERS and MD simulations**

D'Urso, L., Condorelli, M., Puglisi, O., Tempra, C., Lolicato, F., Compagnini, G. & La Rosa, C., 2018, In : Physical Chemistry Chemical Physics. 20, 31, p. 20588-20596 9 p.



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

**Stable carbon isotopic composition of peat columns, subsoil and vegetation on natural and forestry-drained boreal peatlands**

Nykänen, H., Mpamah, P. A. & Rissanen, A. J., 2018, In : *Isotopes in Environmental and Health Studies*. 54, 6  
Research output: Contribution to journal › Article › Scientific › peer-review

**Optical frequency comb photoacoustic spectroscopy**

Sadiq, I., Mikkonen, T., Vainio, M., Toivonen, J. & Foltynowicz, A., 2018, In : *Physical Chemistry Chemical Physics*. 20, 44, p. 27849-27855 7 p.

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

**Efficient photon upconversion at remarkably low annihilator concentrations in a liquid polymer matrix: when less is more**

Durandin, N. A., Isokuortti, J., Efimov, A., Vuorimaa-Laukkanen, E., Tkachenko, N. V. & Laaksonen, T., 2018, In : *Chemical Communications*. 54, 99, p. 14029-14032 4 p.

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

**On the molecular optical nonlinearity of halogen-bond-forming azobenzenes**

Virkki, M., Maurice, A., Forni, A., Sironi, M., Dichiarante, V., Brevet, P. F., Metrangolo, P., Kauranen, M. & Priimagi, A., 2018, In : *Physical Chemistry Chemical Physics*. 20, 45, p. 28810-28817 8 p.

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

**Supercritical carbon dioxide treatment of hot dip galvanized steel as a surface treatment before coating**

Saarimaa, V., Kaleva, A., Nikkanen, J-P., Heinonen, S., Levänen, E., Väisänen, P., Markkula, A. & Juhanoja, J., 15 Dec 2017, In : *Surface and Coatings Technology*. 331, p. 137-142 6 p.

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

**Time-Resolved Fluorescence Spectroscopy Reveals Fine Structure and Dynamics of Poly(L-lysine) and Polyethylenimine Based DNA Polyplexes**

Lisitsyna, E. S., Ketola, T-M., Morin-Picardat, E., Liang, H., Hanzlíková, M., Urtti, A., Yliperttula, M. & Vuorimaa-Laukkanen, E., 7 Dec 2017, In : *Journal of Physical Chemistry B*. 121, 48, p. 10782-10792 11 p.

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

**Mapping microscale wetting variations on biological and synthetic water-repellent surfaces**

Liimatainen, V., Vuckovac, M., Jokinen, V., Sariola, V., Hokkanen, M. J., Zhou, Q. & Ras, R. H. A., 1 Dec 2017, In : *Nature Communications*. 8, 1, 1798.

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

**Oxygen and water vapor transmission rates of starch-poly(vinyl alcohol) barrier coatings for flexible packaging paper**

Christophliemk, H., Johansson, C., Ullsten, H. & Järnström, L., 1 Dec 2017, In : *Progress in Organic Coatings*. 113, p. 218-224 7 p.

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

**Carbazole-based small molecule electron donors: Syntheses, characterization, and material properties**

Sippola, R. J., Hadipour, A., Kastinen, T., Vivo, P., Hukka, T. I., Aernouts, T. & Heiskanen, J. P., 8 Nov 2017, In : *Dyes and Pigments*. 150, p. 79-88 10 p., j.dyepig.2017.11.014.

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

**DoGlycans-Tools for Preparing Carbohydrate Structures for Atomistic Simulations of Glycoproteins, Glycolipids, and Carbohydrate Polymers for GROMACS**

Danne, R., Poojari, C., Martinez-Seara, H., Rissanen, S., Lolicato, F., Róg, T. & Vattulainen, I., 23 Oct 2017, In : *Journal of Chemical Information and Modeling*. 57, 10, p. 2401-2406 6 p.

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

**Starch-poly(vinyl alcohol) barrier coatings for flexible packaging paper and their effects of phase interactions**

Christophliemk, H., Ullsten, H., Johansson, C. & Järnström, L., 1 Oct 2017, In : *Progress in Organic Coatings*. 111, p. 13-22 10 p.

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

#### **Systematic analysis of coating-substrate interactions in the presence of flow localization**

Isakov, M., Matikainen, V., Koivuluoto, H. & May, M., 15 Sep 2017, In : Surface and Coatings Technology. 324, p. 264-280 17 p.

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

#### **Membrane Binding of Recoverin: From Mechanistic Understanding to Biological Functionality**

Timr, Š., Pleskot, R., Kadlec, J., Kohagen, M., Magarkar, A. & Jungwirth, P., 23 Aug 2017, In : ACS Central Science. 3, 8, p. 868-874 7 p.

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

#### **Exhaust emissions of non-road mobile machine: Real-world and laboratory studies with diesel and HVO fuels**

Pirjola, L., Rönkkö, T., Saukko, E., Parviainen, H., Malinen, A., Alanen, J. & Saveljeff, H., 15 Aug 2017, In : Fuel. 202, p. 154-164 11 p.

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

#### **Feed-hopper level estimation and control in cone crushers**

Itävuori, P., Hulthén, E. & Viikko, M., 15 Aug 2017, In : Minerals Engineering. 110, p. 82-95 14 p.

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

#### **Configurational Disorder of Water Hydrogen-Bond Network at the Protein Dynamical Transition**

Rahaman, O., Kalimeri, M., Katava, M., Paciaroni, A. & Sterpone, F., 20 Jul 2017, In : Journal of Physical Chemistry Part B. 121, 28, p. 6792-6798 7 p.

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

#### **Vegetable fillers for electric stimuli responsive elastomers**

Poikelispää, M., Shakun, A., Sarlin, E., Das, A. & Vuorinen, J., 20 Jul 2017, In : Journal of Applied Polymer Science. 134, 28, 45081.

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

#### **Electropolymerized polyazulene as active material in flexible supercapacitors**

Suominen, M., Lehtimäki, S., Yewale, R., Damlin, P., Tuukkanen, S. & Kvarnström, C., 15 Jul 2017, In : Journal of Power Sources. 356, p. 181-190 10 p.

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

#### **Dynamics of a True Moving Bed separation process: Linear model identification and advanced process control**

Nogueira, I. B. R., Ribeiro, A. M., Martins, M. A. F., Rodrigues, A. E., Koivisto, H. & Loureiro, J. M., 30 Jun 2017, In : Journal of Chromatography A. 1504

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

#### **Long-Range Observation of Exciplex Formation and Decay Mediated by One-Dimensional Bridges**

Baek, J., Umeyama, T., Stranius, K., Yamada, H., Tkachenko, N. V. & Imahori, H., 29 Jun 2017, In : Journal of Physical Chemistry C. 121, 25, p. 13952-13961 10 p.

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

#### **Comparison of starch and gelatin hydrogels for non-toxic supercapacitor electrolytes**

Railanmaa, A., Lehtimäki, S. & Lupo, D., 1 Jun 2017, In : Applied Physics A-Materials Science and Processing. 123, 6, 459.

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

#### **Catalytic Activity of AuCu Clusters on MgO(100): Effect of Alloy Composition for CO Oxidation**

Ma, L., Laasonen, K. & Akola, J., 25 May 2017, In : Journal of Physical Chemistry C. 121, 20, p. 10876-10886 11 p.

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

### **Geometric Structure and Chemical Ordering of Large AuCu Clusters: A Computational Study**

Goh, J.-Q., Akola, J. & Ferrando, R., 25 May 2017, In : Journal of Physical Chemistry C. 121, 20, p. 10809-10816 8 p.  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Nematicon-enhanced spontaneous symmetry breaking**

Piccardi, A., Alberucci, A., Kravets, N., Buchnev, O. & Assanto, G., 24 May 2017, In : Molecular Crystals and Liquid Crystals. 649, 1, p. 59-65 7 p.

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

### **Density functional study of structure and dynamics in liquid antimony and Sb<sub>n</sub> clusters**

Jones, R. O., Ahlstedt, O., Akola, J. & Ropo, M., 21 May 2017, In : Journal of Chemical Physics. 146, 19, 194502.

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

### **The effects of calcium and potassium on CO<sub>2</sub> gasification of birch wood in a fluidized bed**

Kramb, J., Gómez-Barea, A., DeMartini, N., Romar, H., Doddapaneni, T. R. K. C. & Kontinen, J., 15 May 2017, In : Fuel. 196, p. 398-407 10 p.

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

### **Photoinduced Electron Injection from Zinc Phthalocyanines into Zinc Oxide Nanorods: Aggregation Effects**

Virkki, K., Hakola, H., Urbani, M., Tejerina, L., Ince, M., Martínez-Díaz, M. V., Torres, T., Golovanova, V., Golovanov, V. & Tkachenko, N. V., 4 May 2017, In : Journal of Physical Chemistry C. 121, 17, p. 9594-9605 12 p.

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

### **Electron microscopic studies of natural gas oxidation catalyst – Effects of thermally accelerated aging on catalyst microstructure**

Honkanen, M., Hansen, T. W., Jiang, H., Kärkkäinen, M., Huuhtanen, M., Heikkinen, O., Kallinen, K., Lahtinen, J., Keiski, R. L., Wagner, J. B. & Vippola, M., 1 May 2017, In : Journal of Catalysis. 349, p. 19-29 11 p.

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

### **Elucidation of Compression-Induced Surface Crystallization in Amorphous Tablets Using Sum Frequency Generation (SFG) Microscopy**

Mah, P. T., Novakovic, D., Saarinen, J., van Landeghem, S., Peltonen, L., Laaksonen, T., Isomäki, A. & Strachan, C. J., May 2017, In : Pharmaceutical Research. 34, 5, p. 957-970 14 p.

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

### **Hexaphyrin as a Potential Theranostic Dye for Photothermal Therapy and <sup>19</sup>F Magnetic Resonance Imaging**

Higashino, T., Nakatsuji, H., Fukuda, R., Okamoto, H., Imai, H., Matsuda, T., Tochio, H., Shirakawa, M., Tkachenko, N. V., Hashida, M., Murakami, T. & Imahori, H., 24 Mar 2017, In : ChemBioChem. 18, 10, p. 951-959 9 p.

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

### **Calcium Directly Regulates Phosphatidylinositol 4,5-Bisphosphate Headgroup Conformation and Recognition**

Bilkova, E., Pleskot, R., Rissanen, S., Sun, S., Czogalla, A., Cwiklik, L., Róg, T., Vattulainen, I., Cremer, P. S., Jungwirth, P. & Coskun, Ü., 22 Mar 2017, In : Journal of the American Chemical Society. 139, 11, p. 4019-4024 6 p.

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

### **Hierarchical Self-Assembly of Halogen-Bonded Block Copolymer Complexes into Upright Cylindrical Domains**

Milani, R., Houbenov, N., Fernandez-Palacio, F., Cavallo, G., Luzio, A., Haataja, J., Giancane, G., Saccone, M., Priimägi, A., Metrangolo, P. & Ikkala, O., 9 Mar 2017, In : Chem. 2, 3, p. 417-426 10 p.

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

### **Membrane cholesterol access into a G-protein-coupled receptor**

Guixà-González, R., Albasanz, J. L., Rodríguez-Espigares, I., Pastor, M., Sanz, F., Martí-Solano, M., Manna, M., Martínez-Seara, H., Hildebrand, P. W., Martín, M. & Selent, J., 21 Feb 2017, In : Nature Communications. 8, 14505.

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

### **Magnetic routing of light-induced waveguides**

Izdebskaya, Y., Shvedov, V., Assanto, G. & Krolikowski, W., 15 Feb 2017, In : Nature Communications. 8, 14452.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Benchmarking DFT methods with small basis sets for the calculation of halogen-bond strengths**

Siiskonen, A. & Priimägi, A., 1 Feb 2017, In : Journal of Molecular Modeling. 23, 2, 50.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Polarization resolved photoluminescence in GaAs<sub>1-x</sub>Bi<sub>x</sub>/GaAs quantum wells**

Balanta, M. A. G., Orsi Gordo, V., Carvalho, A. R. H., Puustinen, J., Alghamdi, H. M., Henini, M., Galeti, H. V. A., Guina, M. & Galvão Gobato, Y., Feb 2017, In : Journal of Luminescence. 182, p. 49-52 4 p.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Architectures and codecs for real-time light field streaming**

Kovács, P. T., Zare, A., Balogh, T., Bregovic, R. & Gotchev, A., 1 Jan 2017, In : Journal of Imaging Science and Technology. 61, 1, 010403.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Improved corrosion properties of Hot Dip Galvanized Steel by nanomolecular silane layers as hybrid interface between zinc and top coatings**

Vuori, L., Ali-Löytty, H., Lahtonen, K., Hannula, M., Lehtonen, E., Niu, Y. & Valden, M., 2017, In : Corrosion. 73, 2  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Synthesis, Structural Characterization, Hirshfeld Surface and Antioxidant Activity Analysis of a Novel Organic Cation Antimonate Complex**

Lahbib, I., Valkonen, A., Rzaigui, M. & Smirani, W., 2017, In : Journal of Cluster Science. 28, 4, p. 2239-2252 14 p.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Effects of orientation at the phthalocyanine-CdSe interface on the electron transfer characteristics**

Golovanov, V. V., Nazarchuk, B. V., Golovanova, V. V., Tkachenko, N. V. & Rantala, T. T., 2017, In : Physical Chemistry Chemical Physics. 19, 16, p. 10511-10517 7 p.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **High-resolution coded-aperture design for compressive X-ray tomography using low resolution detectors**

Mojica, E., Pertuz, S. & Arguello, H., 2017, In : Optics Communications. 404, p. 103-109  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Crystallization and sintering of borosilicate bioactive glasses for application in tissue engineering**

Fabert, M., Ojha, N., Erasmus, E., Hannula, M., Hokka, M., Hyttinen, J., Rocherullé, J., Sigalas, I. & Massera, J., 2017, In : Journal of Materials Chemistry B. 5, 23, p. 4514-4525 12 p.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Two cations, two mechanisms: Interactions of sodium and calcium with zwitterionic lipid membranes**

Javanainen, M., Melcrová, A., Magarkar, A., Jurkiewicz, P., Hof, M., Jungwirth, P. & Martinez-Seara, H., 2017, In : Chemical Communications. 53, 39, p. 5380-5383 4 p.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Supramolecular control of liquid crystals by doping with halogen-bonding dyes**

Vapaavuori, J., Siiskonen, A., Dichiarante, V., Forni, A., Saccone, M., Pilati, T., Pellerin, C., Shishido, A., Metrangolo, P. & Priimägi, A., 2017, In : RSC Advances. 7, 64, p. 40237-40242 6 p.  
Research output: Contribution to journal › Article › Scientific › peer-review

### **Photoresponsive ionic liquid crystals assembled: Via halogen bond: En route towards light-controllable ion transporters**

Saccone, M., Palacio, F. F., Cavallo, G., Dichiarante, V., Virkki, M., Terraneo, G., Priimägi, A. & Metrangolo, P., 2017, In : Faraday Discussions. 203, p. 407-422 16 p.  
Research output: Contribution to journal › Article › Scientific › peer-review

**Photophysical properties of porphyrin dimer-single-walled carbon nanotube linked systems**

Baek, J., Umeyama, T., Mizuno, S., Tkachenko, N. V. & Imahori, H., 2017, In : Journal of Physical Chemistry C. 121, 39  
Research output: Contribution to journal > Article > Scientific > peer-review

**Design of a 25 MWe Solar Thermal Power Plant in Iran with Using Parabolic Trough Collectors and a Two-Tank Molten Salt Storage System**

Kordmahaleh, A. A., Naghashzadegan, M., Javaherdeh, K. & Khoshgoftar, M., 2017, In : International Journal of Photoenergy. 2017, 4210184.  
Research output: Contribution to journal > Article > Scientific > peer-review

**Particle emissions characterization from a medium-speed marine diesel engine with two fuels at different sampling conditions**

Ntziachristos, L., Saukko, E., Lehtoranta, K., Rönkkö, T., Timonen, H., Simonen, P., Karjalainen, P. & Keskinen, J., 15 Dec 2016, In : Fuel. 186, p. 456-465 10 p.  
Research output: Contribution to journal > Article > Scientific > peer-review

**Optimization of HVOF Cr<sub>3</sub>C<sub>2</sub>-NiCr coating for increased fatigue performance**

Varis, T., Suhonen, T., Calonius, O., Čuban, J. & Pietola, M., 15 Nov 2016, In : Surface and Coatings Technology. 305, p. 123-131 9 p.  
Research output: Contribution to journal > Article > Scientific > peer-review

**Collective excitations and viscosity in liquid Bi**

Ropo, M., Akola, J. & Jones, R. O., 14 Nov 2016, In : Journal of Chemical Physics. 145, 18, 184502.  
Research output: Contribution to journal > Article > Scientific > peer-review

**Improvement of actuation performance of dielectric elastomers by barium titanate and carbon black fillers**

Poikelispää, M., Shakun, A., Das, A. & Vuorinen, J., 10 Nov 2016, In : Journal of Applied Polymer Science. 133, 42, 44116.  
Research output: Contribution to journal > Article > Scientific > peer-review

**London Hybrid Exposure Model: Improving Human Exposure Estimates to NO<sub>2</sub> and PM<sub>2.5</sub> in an Urban Setting**

Smith, J. D., Mitsakou, C., Kitwiroon, N., Barratt, B. M., Walton, H. A., Taylor, J. G., Anderson, H. R., Kelly, F. J. & Beevers, S. D., 1 Nov 2016, In : Environmental Science and Technology. 50, 21, p. 11760-11768 9 p.  
Research output: Contribution to journal > Article > Scientific > peer-review

**Grain orientation dependent Nb-Ti microalloying mediated surface segregation on ferritic stainless steel**

Ali-Löytty, H., Hannula, M., Honkanen, M., Östman, K., Lahtonen, K. & Valden, M., Nov 2016, In : Corrosion Science. 112, p. 204-213  
Research output: Contribution to journal > Article > Scientific > peer-review

**UPS and DFT investigation of the electronic structure of gas-phase trimesic acid**

Reisberg, L., Pärna, R., Kikas, A., Kuusik, I., Kisand, V., Hirsimäki, M., Valden, M. & Nömmiste, E., Nov 2016, In : Journal of Electron Spectroscopy and Related Phenomena. 213, p. 11-16 6 p.  
Research output: Contribution to journal > Article > Scientific > peer-review

**Increased survival rate by local release of diclofenac in a murine model of recurrent oral carcinoma**

Will, O. M., Purcz, N., Chalaris, A., Heneweer, C., Boretius, S., Purcz, L., Nikkola, L., Ashammakhi, N., Kalthoff, H., Glüer, C. C., Wiltfang, J., Açil, Y. & Tiwari, S., 12 Oct 2016, In : International Journal of Nanomedicine. 11, p. 5311-5321 11 p.  
Research output: Contribution to journal > Article > Scientific > peer-review

**Elimination of arsenic-containing emissions from gasification of chromated copper arsenate wood**

Kramb, J., Konttinen, J., Backman, R., Salo, K. & Roberts, M., 1 Oct 2016, In : Fuel. 181, p. 319-324 6 p.  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Controlling the motion of multiple objects on a Chladni plate**

Zhou, Q., Sariola, V., Latifi, K. & Liimatainen, V., 9 Sep 2016, In : Nature Communications. 7, 12764.  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Polyarginine Interacts More Strongly and Cooperatively than Polylysine with Phospholipid Bilayers**

Robison, A. D., Sun, S., Poyton, M. F., Johnson, G. A., Pellois, J. P., Jungwirth, P., Vazdar, M. & Cremer, P. S., 8 Sep 2016, In : Journal of Physical Chemistry Part B. 120, 35, p. 9287-9296 10 p.  
Research output: Contribution to journal > Article > Scientific > peer-review

### **3D micro-nano structured hybrid scaffolds: An investigation into the role of nanofiber coating on viability, proliferation and differentiation of seeded mesenchymal stem cells**

Pilehrood, M. K., Atashi, A., Sadeghi-Aliabadi, H., Nousiainen, P. & Harlin, A., 1 Sep 2016, In : Journal Nanoscience and Nanotechnology. 16, 9, p. 9000-9007 8 p.  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Detergent impurity effect on recycled HDPE: Properties after repetitive processing**

Mylläri, V., Hartikainen, S., Poliakova, V., Anderson, R., Jönkkäri, I., Pasanen, P., Andersson, M. & Vuorinen, J., 15 Aug 2016, In : Journal of Applied Polymer Science. 133, 31, 43766.  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Buckling Behavior of Cold-Formed Studs with Thermal Perforations**

Garifullin, M., Sinelnikov, A., Bronzova, M., Kovacic, B. & Kamnik, R., 11 Aug 2016, In : MATEC Web of Conferences. 73, 04011.  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Reinforced chloroprene rubber by in situ generated silica particles: Evidence of bound rubber on the silica surface**

Kapgate, B. P., Das, C., Das, A., Basu, D., Wiessner, S., Reuter, U. & Heinrich, G., 10 Aug 2016, In : Journal of Applied Polymer Science. 133, 30, 43717.  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Spontaneous formation of three-dimensionally ordered Bi-rich nanostructures within GaAs<sub>1-x</sub>Bi<sub>x</sub>/GaAs quantum wells**

Luna, E., Wu, M., Hanke, M., Puustinen, J., Guina, M. & Trampert, A., 1 Jul 2016, In : Nanotechnology. 27, 32, 325603.  
Research output: Contribution to journal > Article > Scientific > peer-review

### **The Influence of Phosphorus Exposure on a Natural-Gas-Oxidation Catalyst**

Kärkkäinen, M., Kolli, T., Honkanen, M., Heikkinen, O., Väliheikki, A., Huuhtanen, M., Kallinen, K., Lahtinen, J., Vippola, M. & Keiski, R. L., 1 Jul 2016, In : Topics in Catalysis. 59, 10-12, p. 1044-1048 5 p.  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Structurally Controlled Dynamics in Azobenzene-Based Supramolecular Self-Assemblies in Solid State**

Poutanen, M., Ikkala, O. & Priimägi, A., 14 Jun 2016, In : Macromolecules. 49, 11, p. 4095-4101 7 p.  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Development of Magnetic Losses During Accelerated Corrosion Tests for Nd-Fe-B Magnets Used in Permanent Magnet Generators**

Isotahdon, E., Huttunen-Saarivirta, E. & Kuokkala, V-T., 1 Jun 2016, In : Corrosion. 72, 6, p. 732-741 10 p.  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Robust statistical approaches for RSS-based floor detection in indoor localization**

Razavi, A., Valkama, M. & Lohan, E. S., 1 Jun 2016, In : Sensors. 16, 6, 793.  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Effect of incorporation of CdS NPs on performance of PTB7: PCBM organic solar cells**

Sharma, R., Bhalerao, S. & Gupta, D., 1 Jun 2016, In : Organic Electronics: physics, materials, applications. 33, p. 274-280 7 p.  
Research output: Contribution to journal > Article > Scientific > peer-review

**Optical Projection Tomography Technique for Image Texture and Mass Transport Studies in Hydrogels Based on Gellan Gum**

Soto, A. M., Koivisto, J. T., Parraga, J. E., Silva-Correia, J., Oliveira, J. M., Reis, R. L., Kellomäki, M., Hyttinen, J. & Figueiras, E., 24 May 2016, In : *Langmuir*. 32, 20, p. 5173-5182 10 p.

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

**Lipid-assisted protein transport: A diffusion-reaction model supported by kinetic experiments and molecular dynamics simulations**

La Rosa, C., Scalisi, S., Lolicato, F., Pannuzzo, M. & Raudino, A., 14 May 2016, In : *Journal of Chemical Physics*. 144, 18, 184901.

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

**Effect of Hole Transporting Material on Charge Transfer Processes in Zinc Phthalocyanine Sensitized ZnO Nanorods**

Hakola, H., Sariola-Leikas, E., Efimov, A. & Tkachenko, N. V., 21 Apr 2016, In : *Journal of Physical Chemistry C*. 120, 13, p. 7044-7051 8 p.

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

**Influence of heat treatment on the abrasive wear resistance of a Cr<sub>3</sub>C<sub>2</sub>NiCr coating deposited by an ethene-fuelled HVOF spray process**

Janka, L., Norpoth, J., Trache, R. & Berger, L. M., 15 Apr 2016, In : *Surface and Coatings Technology*. 291, p. 444-451 8 p.

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

**Coordination networks incorporating halogen-bond donor sites and azobenzene groups**

Fernandez-Palacio, F., Saccone, M., Priimägi, A., Terraneo, G., Pilati, T., Metrangolo, P. & Resnati, G., 7 Apr 2016, In : *CrystEngComm*. 18, 13, p. 2251-2257 7 p.

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

**Strain rate change tests with the Split Hopkinson Bar method**

Isakov, M., Kokkonen, J., Östman, K. & Kuokkala, V-T., 1 Apr 2016, In : *European Physical Journal. Special Topics*. 225, 2, p. 231-242

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

**DFT simulations and microkinetic modelling of 1-pentyne hydrogenation on Cu<sub>20</sub> model catalysts**

Ma, L., Melander, M., Weckman, T., Lipasti, S., Laasonen, K. & Akola, J., 1 Apr 2016, In : *Journal of Molecular Graphics and Modelling*. 65, p. 61-70 10 p.

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

**Microwave assisted laser-induced breakdown spectroscopy at ambient conditions**

Viljanen, J., Sun, Z. & Alwahabi, Z. T., 1 Apr 2016, In : *Spectrochimica Acta Part B: Atomic Spectroscopy*. 118, p. 29-36 8 p.

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

**Metal chalcogenide quantum dots: Biotechnological synthesis and applications**

Mal, J., Nancharaiyah, Y. V., Van Hullebusch, E. D. & Lens, P. N. L., Apr 2016, In : *RSC Advances*. 6, 47, p. 41477-41495 19 p.

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

**Long-Lived Triplet Excited States of Bent-Shaped Pentacene Dimers by Intramolecular Singlet Fission**

Sakuma, T., Sakai, H., Araki, Y., Mori, T., Wada, T., Tkachenko, N. V. & Hasobe, T., 31 Mar 2016, In : *Journal of Physical Chemistry A*. 120, 11, p. 1867-1875 9 p.

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

**Stability and Function at High Temperature. What Makes a Thermophilic GTPase Different from Its Mesophilic Homologue**

Katava, M., Kalimeri, M., Stirnemann, G. & Sterpone, F., 17 Mar 2016, In : *Journal of Physical Chemistry Part B*. 120, 10, p. 2721-2730 10 p.

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

#### **HPLC-SEC: a new approach to characterise complex wastewater effluents**

Szabo, H. M., Lepistö, R. & Tuhkanen, T., 19 Feb 2016, In : International Journal of Environmental Analytical Chemistry. 96, 3, p. 257-270 14 p.

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

#### **Phenothiazine and carbazole substituted pyrene based electroluminescent organic semiconductors for OLED devices**

Salunke, J. K., Wong, F. L., Feron, K., Manzhos, S., Lo, M. F., Shinde, D., Patil, A., Lee, C. S., Roy, V. A. L., Sonar, P. & Wadgaonkar, P. P., 7 Feb 2016, In : Journal of Materials Chemistry C. 4, 5, p. 1009-1018 10 p.

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

#### **Ambient-Pressure XPS Study of a Ni-Fe Electrocatalyst for the Oxygen Evolution Reaction**

Ali-Löyty, H., Louie, M. W., Singh, M. R., Li, L., Sanchez Casalongue, H. G., Ogasawara, H., Crumlin, E. J., Liu, Z., Bell, A. T., Nilsson, A. & Friebel, D., 4 Feb 2016, In : Journal of Physical Chemistry C. 120, 4, p. 2247-2253 7 p.

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

#### **Guanidinium Pairing Facilitates Membrane Translocation**

Allolio, C., Baxova, K., Vazdar, M. & Jungwirth, P., 14 Jan 2016, In : Journal of Physical Chemistry Part B. 120, 1, p. 143-153 11 p.

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

#### **Physical and Chemical Characterization of Real-World Particle Number and Mass Emissions from City Buses in Finland**

Pirjola, L., Dittrich, A., Niemi, J. V., Saarikoski, S., Timonen, H., Kuuluvainen, H., Järvinen, A., Kousa, A., Rönkkö, T. & Hillamo, R., 5 Jan 2016, In : Environmental Science and Technology. 50, 1, p. 294-304 11 p.

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

#### **Heat capacities of crystalline and glassy lithium metaphosphate up to the transition region**

Rocherullé, J., Massera, J., Oudadesse, H., Calvez, L., Trolès, J. & Zhang, X. H., 2016, In : Journal of Thermal Analysis and Calorimetry. 123, 1, p. 401-407 7 p.

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

#### **Thermal desorption of molecular oxygen from SnO<sub>2</sub> (110) surface: Insights from first-principles calculations**

Golovanov, V., Golovanova, V. & Rantala, T. T., 2016, In : Journal of Physics and Chemistry of Solids. 89, p. 15-22 8 p.

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**

Higashino, T., Yamada, T., Yamamoto, M., Furube, A., Tkachenko, N. V., Miura, T., Kobori, Y., Jono, R., Yamashita, K. & Imahori, H., 2016, In : Angewandte Chemie (International Edition). 55, 2, p. 629-633

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

#### **Preferential adsorption of Cu in a multi-metal mixture onto biogenic elemental selenium nanoparticles**

Jain, R., Dominic, D., Jordan, N., Rene, E. R., Weiss, S., van Hullebusch, E. D., Hübner, R. & Lens, P. N. L., 2016, In : Chemical Engineering Journal. 284, p. 917-925

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

#### **A Three-Component Assembly Promoted by Boronic Acids Delivers a Modular Fluorophore Platform (BASHY Dyes)**

Santos, F. M. F., Rosa, J. N., Candeias, N. R., Carvalho, C. P., Matos, A. I., Ventura, A. E., Florindo, H. F., Silva, L. C., Pischel, U. & Gois, P. M. P., 2016, In : Chemistry: A European Journal. 22, 5, p. 1631-1637

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

#### **The electrooxidation-induced structural changes of gold di-superatomic molecules: Au<sub>23</sub> vs. Au<sub>25</sub>**

Matsuo, S., Yamazoe, S., Goh, J-Q., Akola, J. & Tsukuda, T., 2016, In : Physical Chemistry Chemical Physics. 18, 6, p. 4822-4827 6 p.

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



### **Cholesterol oxidation products and their biological importance**

Kulig, W., Cwiklik, L., Jurkiewicz, P., Rog, T. & Vattulainen, I., 2016, In : Chemistry and Physics of Lipids. 199, p. 144-160 17 p.

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

### **High-Yield Excited Triplet States in Pentacene Self-Assembled Monolayers on Gold Nanoparticles through Singlet Exciton Fission**

Kato, D., Sakai, H., Tkachenko, N. V. & Hasobe, T., 2016, In : Angewandte Chemie (International Edition). 55, 17, p. 5230-5234

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

### **Superfluorinated Ionic Liquid Crystals Based on Supramolecular, Halogen-Bonded Anions**

Cavallo, G., Terraneo, G., Monfredini, A., Saccone, M., Priimägi, A., Pilati, T., Resnati, G., Metrangolo, P. & Bruce, D. W., 2016, In : Angewandte Chemie (International Edition). 55, 21, p. 6300-6304

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

### **Compatibilization of natural rubber/nitrile rubber blends by sol-gel nano-silica generated by in situ method**

Bansod, N. D., Kapgade, B. P., Das, C., Das, A., Basu, D. & Debnath, S. C., 2016, In : JOURNAL OF SOL-GEL SCIENCE AND TECHNOLOGY. 80, 2, p. 548-559 12 p.

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

### **Controllable Electronic Structures and Photoinduced Processes of Bay-Linked Perylene-3,9-dimide Dimers and a Ferrocene-Linked Triad**

Horinouchi, H., Sakai, H., Araki, Y., Sakanoue, T., Takenobu, T., Wada, T., Tkachenko, N. V. & Hasobe, T., 2016, In : Chemistry: A European Journal. 22, 28, p. 9631-9641

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

### **Fire-safe and environmentally friendly nanocomposites based on layered double hydroxides and ethylene propylene diene elastomer**

Basu, D., Das, A., Wang, D. Y., George, J. J., Stöckelhuber, K. W., Boldt, R., Leuteritz, A. & Heinrich, G., 2016, In : RSC Advances. 6, 31, p. 26425-26436 12 p.

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

### **Alginate microgels created by selective coalescence between core drops paired with an ultrathin shell**

Lee, T. Y., Ramasamy, P., Oh, Y. K., Lee, K. & Kim, S. H., 2016, In : Journal of Materials Chemistry B. 4, 19, p. 3232-3238 7 p.

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

### **Decoding the Morphological Diversity in Two Dimensional Crystalline Porous Polymers by Core Planarity Modulation**

Halder, A., Kandambeth, S., Biswal, B. P., Kaur, G., Roy, N. C., Addicoat, M., Salunke, J. K., Banerjee, S., Vanka, K., Heine, T., Verma, S. & Banerjee, R., 2016, In : Angewandte Chemie (International Edition). 55, 27, p. 7806-7810 5 p.

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

### **Photoresponsive liquid-crystalline polymer films bilayered with an inverse opal structure**

Akamatsu, N., Aizawa, M., Tatsumi, R., Hisano, K., Priimägi, A. & Shishido, A., 2016, In : JOURNAL OF PHOTOPOLYMER SCIENCE AND TECHNOLOGY. 29, 1, p. 145-148 4 p.

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

### **Optical non-contact pH measurement in cell culture with sterilizable, modular parts**

Kattiparambil Rajan, D., Patrikoski, M., Verho, J., Sivula, J., Ihalainen, H., Miettinen, S. & Lekkala, J., 2016, In : Talanta. 161, p. 755-761 6 p.

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

### **On describing the optoelectronic characteristics of poly(benzodithiophene-: Co -quinoxaline)-fullerene complexes: The influence of optimally tuned density functionals**

Kastinen, T., Niskanen, M., Risko, C., Cramariuc, O. & Hukka, T. I., 2016, In : Physical Chemistry Chemical Physics. 18, 39, p. 27654-27670 17 p.

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

**Enhanced adsorption of orthophosphate and copper onto hydrochar derived from sewage sludge by KOH activation**

Spataru, A., Jain, R., Chung, J. W., Gerner, G., Krebs, R. & Lens, P. N. L., 2016, In : RSC Advances. 6, 104, p. 101827-101834 8 p.

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

**Nonlinear transmittance and optical power limiting in magnesium ferrite nanoparticles: effects of laser pulsewidth and particle size**

Perumbilavil, S., Sridharan, K., Abraham, A. R., Janardhanan, H. P., Kalarikkal, N. & Philip, R., 2016, In : RSC Advances. 6, 108, p. 106754-106761 8 p.

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

**Synthesis, crystal structure, physico-chemical characterization and dielectric properties of a new hybrid material, 1-Ethylpiperazine-1,4-dium tetrachlorocadmate**

Dhieb, A. C., Valkonen, A., Rzaigui, M. & Smirani, W., 15 Dec 2015, In : Journal of Molecular Structure. 1102, p. 50-56 7 p.

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

**The formation and physical properties of the particle emissions from a natural gas engine**

Alanen, J., Saukko, E., Lehtoranta, K., Murtonen, T., Timonen, H., Hillamo, R., Karjalainen, P., Kuuluvainen, H., Harra, J., Keskinen, J. & Rönkkö, T., 15 Dec 2015, In : Fuel. 162, p. 155-161 7 p.

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

**Modeling carbon dioxide transport in PDMS-based microfluidic cell culture devices**

Mäki, A. J., Peltokangas, M., Kreuzer, J., Auvinen, S. & Kallio, P., 1 Dec 2015, In : Chemical Engineering Science. 137, p. 515-524 10 p.

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

**Differential basal-to-apical accessibility of lamin A/C epitopes in the nuclear lamina regulated by changes in cytoskeletal tension**

Ihalainen, T. O., Aires, L., Herzog, F. A., Schwartlander, R., Moeller, J. & Vogel, V., 1 Dec 2015, In : Nature Materials. 14, 12, p. 1252-1261 10 p.

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

**Graphene-intercalated Fe<sub>2</sub>O<sub>3</sub>/TiO<sub>2</sub> heterojunctions for efficient photoelectrolysis of water**

Kaouk, A., Ruoko, T. P., Gönüllü, Y., Kaunisto, K., Mettenböcker, A., Gurevich, E., Lemmetyinen, H., Ostendorf, A. & Mathur, S., 13 Nov 2015, In : RSC Advances. 5, 123, p. 101401-101407 7 p.

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

**Tri-functionality of Fe<sub>3</sub>O<sub>4</sub>-embedded carbon microparticles in microalgae harvesting**

Seo, J. Y., Lee, K., Ramasamy, P., Kim, B., Lee, S. Y., Oh, Y. K. & Park, S. B., 5 Nov 2015, In : Chemical Engineering Journal. 280, p. 206-214 9 p.

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

**Effect of rubber polarity on selective wetting of carbon nanotubes in ternary blends**

Le, H. H., Parsaker, M., Sriharish, M. N., Henning, S., Menzel, M., Wießner, S., Das, A., Do, Q. K., Heinrich, G. & Radosch, H. J., 1 Nov 2015, In : Express Polymer Letters. 9, 11, p. 960-971 12 p.

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

**Comparison of different cationized proteins as biomaterials for nanoparticle-based ocular gene delivery**

Zorzi, G. K., Párraga, J. E., Seijo, B. & Sanchez, A., 1 Nov 2015, In : Colloids and Surfaces B: Biointerfaces. 135, p. 533-541 9 p.

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

### **Submolecular Plasticization Induced by Photons in Azobenzene Materials**

Vapaavuori, J., Laventure, A., Bazuin, C. G., Lebel, O. & Pellerin, C., 28 Oct 2015, In : Journal of the American Chemical Society. 137, 42, p. 13510-13517 8 p.

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

### **Photomechanical Energy Transfer to Photopassive Polymers through Hydrogen and Halogen Bonds**

Vapaavuori, J., Heikkinen, I. T. S., Dichiarante, V., Resnati, G., Metrangolo, P., Sabat, R. G., Bazuin, C. G., Priimagi, A. & Pellerin, C., 27 Oct 2015, In : Macromolecules. 48, 20, p. 7535-7542 8 p.

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

### **In Situ Photocontrol of Block Copolymer Morphology during Dip-Coating of Thin Films**

Vapaavuori, J., Grosrenaud, J., Pellerin, C. & Bazuin, C. G., 20 Oct 2015, In : ACS Macro Letters. 4, 10, p. 1158-1162 5 p.

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

### **Production of sulfonated polyetheretherketone/polypropylene fibers for photoactive textiles**

Mylläri, V., Fatarella, E., Ruzzante, M., Pogni, R., Baratto, M. C., Skrifvars, M., Syrjälä, S. & Järvelä, P., 1 Oct 2015, In : Journal of Applied Polymer Science. 132, 39, 42595.

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

### **Atomic-level characterization of transport cycle thermodynamics in the glycerol-3-phosphate: Phosphate antiporter**

Moradi, M., Enkavi, G. & Tajkhorshid, E., 29 Sep 2015, In : Nature Communications. 6, 8393.

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

### **PIP2 and Talin Join Forces to Activate Integrin**

Orlowski, A., Kukkurainen, S., Pöyry, A., Rissanen, S., Vattulainen, I., Hytönen, V. P. & Róg, T., 24 Sep 2015, In : Journal of Physical Chemistry Part B. 119, 38, p. 12381-12389 9 p.

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

### **Construction of an Interconnected Nanostructured Carbon Black Network: Development of Highly Stretchable and Robust Elastomeric Conductors**

Bhagavatheswaran, E. S., Parsekar, M., Das, A., Le, H. H., Wiessner, S., Stöckelhuber, K. W., Schmaucks, G. & Heinrich, G., 17 Sep 2015, In : Journal of Physical Chemistry C. 119, 37, p. 21723-21731 9 p.

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

### **Effect of spraying parameters on the microstructural and corrosion properties of HVOF-sprayed Fe-Cr-Ni-B-C coatings**

Milanti, A., Matikainen, V., Koivuluoto, H., Bolelli, G., Lusvardi, L. & Vuoristo, P., 15 Sep 2015, In : Surface and Coatings Technology. 277, p. 81-90 10 p.

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

### **Superatom Model for Ag-S Nanocluster with Delocalized Electrons**

Goh, J. Q. & Akola, J., 10 Sep 2015, In : Journal of Physical Chemistry C. 119, 36, p. 21165-21172 8 p.

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

### **Molecular Design of Light-Responsive Hydrogels, for in Situ Generation of Fast and Reversible Valves for Microfluidic Applications**

Ter Schiphorst, J., Coleman, S., Stumpel, J. E., Ben Azouz, A., Diamond, D. & Schenning, A. P. H. J., 8 Sep 2015, In : Chemistry of Materials. 27, 17, p. 5925-5931 7 p.

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

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

Frankberg, E. J., George, L., Efimov, A., Honkanen, M., Pessi, J. & Levänen, E., 2 Sep 2015, In : Fullerenes Nanotubes and Carbon Nanostructures. 23, 9, p. 755-759 5 p.

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

### **Unintentional boron contamination of MBE-grown GaInP/AlGaInP quantum wells**

Tukiainen, A., Likonen, J., Toikkanen, L. & Leinonen, T., 1 Sep 2015, In : Journal of Crystal Growth. 425, p. 60-63  
Research output: Contribution to journal > Article > Scientific > peer-review

### **Searching for a robust strategy for minimizing alkali chlorides in fluidized bed boilers during burning of high SRF-energy-share fuel**

Bajamundi, C. J. E., Vainikka, P., Hedman, M., Silvennoinen, J., Heinanen, T., Taipale, R. & Konttinen, J., 1 Sep 2015, In : Fuel. 155, p. 25-36 12 p.

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

### **How large are nonadiabatic effects in atomic and diatomic systems?**

Yang, Y., Kylänpää, I., Tubman, N. M., Krogel, J. T., Hammes-Schiffer, S. & Ceperley, D. M., Sep 2015, In : Journal of Chemical Physics. 143, 12, 124308.

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

### **Fe<sub>2</sub>O<sub>3</sub>-TiO<sub>2</sub> nanosystems by a hybrid PE-CVD/ALD approach: controllable synthesis, growth mechanism, and photocatalytic properties**

Barreca, D., Carraro, G., Warwick, M. E. A., Kaunisto, K., Gasparotto, A., Gombac, V., Sada, C., Turner, S., Van Tendeloo, G., Maccato, C. & Fornasiero, P., 28 Aug 2015, In : CrystEngComm. 17, 32, p. 6219-6226 8 p.

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

### **Effects of thinning and heating for TiO<sub>2</sub>/AlInP junctions**

Mäkelä, J., Tuominen, M., Yasir, M., Polojärvi, V., Aho, A., Tukiainen, A., Kuzmin, M., Punkkinen, M. P. J., Laukkanen, P., Kokko, K. & Guina, M., 24 Aug 2015, In : Journal of Electron Spectroscopy and Related Phenomena. 205, p. 6-9 4 p.

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**

Lepcha, A., Maccato, C., Mettenböcker, 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., 20 Aug 2015, In : Journal of Physical Chemistry C. 119, 33, p. 18835-18842 8 p.

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

### **Influence of relative humidity and physical load during storage on dustiness of inorganic nanomaterials: implications for testing and risk assessment**

Levin, M., Rojas, E., Vanhala, E., Vippola, M., Liguori, B., Kling, K. I., Koponen, I. K., Mølhav, K., Tuomi, T., Gregurec, D., Moya, S. & Jensen, K. A., 14 Aug 2015, In : Journal of Nanoparticle Research. 17, 8, 337.

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

### **Effect of Phosphatidic Acid on Biomembrane: Experimental and Molecular Dynamics Simulations Study**

Kwolek, U., Kulig, W., Wydro, P., Nowakowska, M., Róg, T. & Kepczynski, M., 6 Aug 2015, In : Journal of Physical Chemistry Part B. 119, 31, p. 10042-10051 10 p.

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

### **Formation and stability of carbon nanotube network in natural rubber: Effect of non-rubber components**

Le, H. H., Pham, T., Henning, S., Klehm, J., Wießner, S., Stöckelhuber, K. W., Das, A., Hoang, X. T., Do, Q. K., Wu, M., Vennemann, N., Heinrich, G. & Radusch, H. J., 5 Aug 2015, In : Polymer. 73, p. 111-121 11 p., 18004.

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

### **Responsive Polymer Photonics**

Stumpel, J. E., 1 Aug 2015, In : ChemistryOpen. 4, 4, p. 533-535 3 p.

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

### **Nonlinear Optical Properties of Fluorescent Dyes Allow for Accurate Determination of Their Molecular Orientations in Phospholipid Membranes**

Timr, Š., Brabec, J., Bondar, A., Ryba, T., Železný, M., Lazar, J. & Jungwirth, P., 30 Jul 2015, In : Journal of Physical Chemistry Part B. 119, 30, p. 9706-9716 11 p.

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

#### **High quality sub-10 nm graphene nanoribbons by on-chip PS-b-PDMS block copolymer lithography**

Rasappa, S., Caridad, J. M., Schulte, L., Cagliani, A., Borah, D., Morris, M. A., Bøggild, P. & Ndoni, S., 29 Jul 2015, In : RSC Advances. 5, 82, p. 66711-66717 7 p.

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

#### **Quantifying non-ergodic dynamics of force-free granular gases**

Bodrova, A., Chechkin, A. V., Cherstvy, A. G. & Metzler, R., 27 Jul 2015, In : Physical Chemistry Chemical Physics. 17, 34, p. 21791-21798 8 p.

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

#### **Photoinduced Electron Transfer in CdSe/ZnS Quantum Dot-Fullerene Hybrids**

Virkki, K., Demir, S., Lemmetyinen, H. & Tkachenko, N. V., 23 Jul 2015, In : Journal of Physical Chemistry C. 119, 31, p. 17561-17572 12 p.

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

#### **Role of Internal Water on Protein Thermal Stability: The Case of Homologous G Domains**

Rahaman, O., Kalimeri, M., Melchionna, S., Hénin, J. & Sterpone, F., 23 Jul 2015, In : Journal of Physical Chemistry Part B. 119, 29, p. 8939-8949 11 p.

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

#### **Electricity production by a microbial fuel cell fueled by brewery wastewater and the factors in its membrane deterioration**

Çetinkaya, A. Y., Köroğlu, E. O., Demir, N. M., Baysoy, D. Y., Özkaya, B. & Çakmakçı, M., 20 Jul 2015, In : Chinese Journal of Catalysis. 36, 7, p. 1068-1076 9 p.

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

#### **Lithography-free oxide patterns as templates for self-catalyzed growth of highly uniform GaAs nanowires on Si(111)**

Hakkarainen, T. V., Schramm, A., Mäkelä, J., Laukkanen, P. & Guina, M., 18 Jul 2015, In : Nanotechnology. 26, 27, p. 275301.

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

#### **Measuring optical anisotropy in poly(3,4-ethylene dioxythiophene): poly(styrene sulfonate) films with added graphene**

Isoniemi, T., Tuukkanen, S., Cameron, D. C., Simonen, J. & Toppari, J. J., 9 Jul 2015, In : Organic Electronics. 25, p. 317-323 7 p.

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

#### **Synthesis and study of electrochemical and optical properties of substituted perylenemonoimides in solutions and on solid surfaces**

Ahmed, Z., George, L., Hiltunen, A., Lemmetyinen, H., Hukka, T. & Efimov, A., 7 Jul 2015, In : Journal of Materials Chemistry A. 3, 25, p. 13332-13339 8 p.

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

#### **Optimal emission enhancement in orthogonal double-pulse laser-induced breakdown spectroscopy**

Sanginés, R., Contreras, V., Sobral, H. & Robledo-Martinez, A., 6 Jul 2015, In : Spectrochimica Acta Part B: Atomic Spectroscopy. 110, p. 139-145 7 p., 4935.

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

#### **A comparison of rheology and FTIR in the study of polypropylene and polystyrene photodegradation**

Mylläri, V., Ruoko, T-P. & Syrjälä, S., 1 Jul 2015, In : Journal of Applied Polymer Science. 132, 28, 6 p., 42246.

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

#### **On the biomaterials for nanostructured ocular therapeutics**

Zorzi, G. K., Párraga, J. E., Seijo, B. & Sánchez, A., 1 Jul 2015, In : Current Organic Chemistry. 19, 15, p. 1443-1459 17 p.

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

**Synthesis and Photophysical Properties of Two Diazaporphyrin-Porphyrin Hetero Dimers in Polar and Nonpolar Solutions**  
Abou-Chahine, F., Fujii, D., Imahori, H., Nakano, H., Tkachenko, N. V., Matano, Y. & Lemmetyinen, H., 18 Jun 2015, In : Journal of Physical Chemistry Part B. 119, 24, p. 7328-7337 10 p.

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

**Catalytic effect of Ca and K on CO<sub>2</sub> gasification of spruce wood char**

Perander, M., DeMartini, N., Brink, A., Kramb, J., Karlström, O., Hemming, J., Moilanen, A., Konttinen, J. & Hupa, M., 15 Jun 2015, In : Fuel. 150, p. 464-472 9 p.

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

**Inverted critical adsorption of polyelectrolytes in confinement**

De Carvalho, S. J., Metzler, R. & Cherstvy, A. G., 14 Jun 2015, In : Soft Matter. 11, 22, p. 4430-4443 14 p.

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

**PEGylated liposomes as carriers of hydrophobic porphyrins**

Dzieciuch, M., Rissanen, S., Szydłowska, N., Bunker, A., Kumorek, M., Jamróz, D., Vattulainen, I., Nowakowska, M., Róg, T. & Kepczynski, M., 4 Jun 2015, In : Journal of Physical Chemistry Part B. 119, 22, p. 6646-6657 12 p.

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

**Equipment for obtaining polymeric nanofibres by electrospinning technology: II. The obtaining of polymeric nanofibers**

Manea, L. R., Cramariuc, B., Popescu, V., Cramariuc, R., Sandu, I. & Cramariuc, O., 1 Jun 2015, In : Materiale Plastice. 52, 2, p. 180-185 6 p.

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

**Polymorph crystal packing effects on charge transfer emission in the solid state**

He, X., Benniston, A. C., Saarenpää, H., Lemmetyinen, H., Tkachenko, N. V. & Baisch, U., 1 Jun 2015, In : Chemical Science. 6, 6, p. 3525-3532 8 p.

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

**Photodiagnostic et chirurgie guidés par la fluorescence**

Mordon, S. & Bourg-Heckly, G., 1 Jun 2015, In : ACTUALITE CHIMIQUE. 397-398, p. 41-45 5 p.

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

**Soft graphoepitaxy for large area directed self-assembly of polystyrene-block-poly(dimethylsiloxane) block copolymer on nanopatterned poss substrates fabricated by nanoimprint lithography**

Borah, D., Rasappa, S., Salaun, M., Zellsman, M., Lorret, O., Lontos, G., Ntetsikas, K., Avgeropoulos, A. & Morris, M. A., 1 Jun 2015, In : Advanced Functional Materials. 25, 22, p. 3425-3432 8 p.

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

**La thérapie photodynamique: État de l'art et perspectives**

Frochot, C., Barberi-Heyob, M., Blanchard-Desce, M., Bolotine, L., Bonneau, S., Jimenez, C. M., Durand, J. O., Lassalle, H. P., Lemerrier, G., Mordon, S., Maillard, P., Sol, V., Vever-Bizet, C. & Vicendo, P., 1 Jun 2015, In : ACTUALITE CHIMIQUE. 397-398, p. 46-50 5 p.

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

**A facile route to synthesis of S-doped TiO<sub>2</sub> nanoparticles for photocatalytic activity**

McManamon, C., O'Connell, J., Delaney, P., Rasappa, S., Holmes, J. D. & Morris, M. A., 30 May 2015, In : Journal of Molecular Catalysis A: Chemical. 406, p. 51-57!

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

**Hydration of hydroxyl and amino groups examined by molecular dynamics and neutron scattering**

Hladílková, J., Fischer, H. E., Jungwirth, P. & Mason, P. E., 28 May 2015, In : Journal of Physical Chemistry Part B. 119, 21, p. 6357-6365 9 p.

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

**Spectral and kinetic characteristics of indotricarbocyanine complexation with albumin**

Kuz'min, V. A., Durandin, N. A., Lisitsyna, E. S., Nekipelova, T. D., Podrugina, T. A., Matveeva, E. D., Proskurnina, M. V. & Zefirov, N. S., 28 May 2015, In : DOKLADY PHYSICAL CHEMISTRY. 462, 1, p. 107-109 3 p.

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

**Effect of melting state on the thermal shock resistance and thermal conductivity of APS ZrO<sub>2</sub>-7.5wt.% Y<sub>2</sub>O<sub>3</sub> coatings**

Song, X., Liu, Z., Suhonen, T., Varis, T., Huang, L., Zheng, X. & Zeng, Y., 25 May 2015, In : Surface and Coatings Technology. 270, p. 132-138 7 p.

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

**Modeling photoionization of aqueous DNA and its components**

Pluhařová, E., Slavíček, P. & Jungwirth, P., 19 May 2015, In : Accounts of Chemical Research. 48, 5, p. 1209-1217 9 p.

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

**Multistep reactions of water with small Pd<sub>n</sub> clusters: A first principles study**

Liang, Y., Ma, L., Wang, J. & Wang, G., 1 May 2015, In : Journal of Theoretical and Computational Chemistry. 14, 3, 1550017.

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

**Energy degradation in photoexcited complexes of indocarbocyanine with albumin**

Kuzmin, V. A., Durandin, N. A., Lisitsyna, E. S., Litvinkova, L. V., Nekipelova, T. D., Podrugina, T. A., Matveeva, E. D., Proskurnina, M. V. & Zefirov, N. S., 1 May 2015, In : HIGH ENERGY CHEMISTRY. 49, 3, p. 211-212 2 p.

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

**Ergodicity breaking and particle spreading in noisy heterogeneous diffusion processes**

Cherstvy, A. G. & Metzler, R., 14 Apr 2015, In : Journal of Chemical Physics. 142, 14, 144105.

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

**Workplace performance of a loose-fitting powered air purifying respirator during nanoparticle synthesis**

Koivisto, A. J., Aromaa, M., Koponen, I. K., Fransman, W., Jensen, K. A., Mäkelä, J. M. & Hämeri, K. J., 9 Apr 2015, In : Journal of Nanoparticle Research. 17, 4

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

**Rate constant and thermochemistry for K + O<sub>2</sub> + N<sub>2</sub> = KO<sub>2</sub> + N<sub>2</sub>**

Sorvajärvi, T., Viljanen, J., Toivonen, J., Marshall, P. & Glarborg, P., 9 Apr 2015, In : Journal of Physical Chemistry A. 119, 14, p. 3329-3336 8 p.

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

**Oxidation of cholesterol does not alter significantly its uptake into high-density lipoprotein particles**

Karilainen, T., Timr, Š., Vattulainen, I. & Jungwirth, P., 2 Apr 2015, In : Journal of Physical Chemistry Part B. 119, 13, p. 4594-4600 7 p.

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

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

Saarikoski, E., Rissanen, M. & Seppälä, J., 30 Mar 2015, In : Carbohydrate Polymers. 119, p. 62-70 9 p.

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

**Effects of fresh lubricant oils on particle emissions emitted by a modern gasoline direct injection passenger car**

Pirjola, L., Karjalainen, P., Heikkilä, J., Saari, S., Tzamkiozis, T., Ntziachristos, L., Kulmala, K., Keskinen, J. & Rönkkö, T., 17 Mar 2015, In : Environmental Science and Technology. 49, 6, p. 3644-3652 9 p.

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

**Tribology of HVOF- and HVOF-sprayed WC-10Co4Cr hardmetal coatings: A comparative assessment**

Bolelli, G., Berger, L. M., Börner, T., Koivuluoto, H., Lusvardi, L., Lyphout, C., Markocsan, N., Matikainen, V., Nylén, P., Sassetelli, P., Trache, R. & Vuoristo, P., 15 Mar 2015, In : Surface and Coatings Technology. 265, p. 125-144 20 p.

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

**High temperature corrosion of thermally sprayed NiCr and FeCr coatings covered with a KCl-K<sub>2</sub>SO<sub>4</sub> salt mixture**

Varis, T., Bankiewicz, D., Yrjas, P., Oksa, M., Suhonen, T., Tuurna, S., Ruusuvuori, K. & Holmström, S., 15 Mar 2015, In : Surface and Coatings Technology. 265, p. 235-243 9 p.

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

**Oxidation of the GaAs semiconductor at the Al<sub>2</sub>O<sub>3</sub>/GaAs junction**

Tuominen, M., Yasir, M., Lång, J., Dahl, J., Kuzmin, M., Mäkelä, J., Punkkinen, M., Laukkanen, P., Kokko, K., Schulte, K., Punkkinen, R., Korpijärvi, V.-M., Polojärvi, V. & Guina, M., 14 Mar 2015, In : Physical Chemistry Chemical Physics. 17, 10, p. 7060-7066 7 p.

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

**CO oxidation catalyzed by neutral and anionic Cu<sub>20</sub> clusters: Relationship between charge and activity**

Ma, L., Melander, M., Laasonen, K. & Akola, J., 14 Mar 2015, In : Physical Chemistry Chemical Physics. 17, 10, p. 7067-7076 10 p.

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

**Synthesis, characterization and solid-state photoluminescence studies of six alkoxy phenylene ethynylene dinuclear palladium(ii) rods**

Figueira, J., Czardybon, W., Mesquita, J. C., Rodrigues, J., Lahoz, F., Russo, L., Valkonen, A. & Rissanen, K., 7 Mar 2015, In : DALTON TRANSACTIONS. 44, 9, p. 4003-4015 13 p.

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

**Resveratrol interferes with the aggregation of membrane-bound human-IAPP: A molecular dynamics study**

Lolicato, F., Raudino, A., Milardi, D. & La Rosa, C., 6 Mar 2015, In : European Journal of Medicinal Chemistry. 92, p. 876-881 6 p.

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

**Crystal structure of 2-methylpiperazine-1,4-dium bis(hydrogen maleate)**

Wecharine, I., Valkonen, A., Rzaigui, M., Sta, W. S. & Smith, G., 1 Mar 2015, In : Acta Crystallographica Section E : Structure Reports Online. 71, 3, p. o193-o194

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

**Exploring the role of stearic acid in modified zinc aluminum layered double hydroxides and their acrylonitrile butadiene rubber nanocomposites**

Eshwaran, S. B., Basu, D., Vaikuntam, S. R., Kutlu, B., Wiessner, S., Das, A., Naskar, K. & Heinrich, G., 1 Mar 2015, In : Journal of Applied Polymer Science. 132, 9, 41539.

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

**Polymer looping is controlled by macromolecular crowding, spatial confinement, and chain stiffness**

Shin, J., Cherstvy, A. G. & Metzler, R., 17 Feb 2015, In : ACS Macro Letters. 4, 2, p. 202-206 5 p.

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

**Neutralized chimeric avidin binding at a reference biosensor surface**

Ray, S., Steven, R. T., Green, F. M., Höök, F., Taskinen, B., Hytönen, V. P. & Shard, A. G., 17 Feb 2015, In : Langmuir. 31, 6, p. 1921-1930 10 p.

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

**Encapsulation of secondary and tertiary ammonium salts by resorcinarenes and pyrogallarenes: The effect of size and charge concentration**

Beyeh, N. K., Pan, F., Valkonen, A. & Rissanen, K., 7 Feb 2015, In : CrystEngComm. 17, 5, p. 1182-1188 7 p.

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

**Second-harmonic generation imaging of semiconductor nanowires with focused vector beams**

Bautista, G., Mäkitalo, J., Chen, Y., Dhaka, V., Grasso, M., Karvonen, L., Jiang, H., Huttunen, M. J., Huhtio, T., Lipsanen, H. & Kauranen, M., 6 Feb 2015, In : Nano Letters. 15, 3, p. 1564-1569 6 p.



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

#### **Sulfonated polyetheretherketone/polypropylene polymer blends for the production of photoactive materials**

Fatarelle, E., Mylläri, V., Ruzzante, M., Pogni, R., Baratto, M. C., Skrifvars, M., Syrjälä, S. & Järvelä, P., 1 Feb 2015, In : Journal of Applied Polymer Science. 132, 8, 41509.

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

#### **Supramolecular hierarchy among halogen and hydrogen bond donors in light-induced surface patterning**

Saccone, M., Dichiarante, V., Forni, A., Goulet-Hanssens, A., Cavallo, G., Vapaavuori, J., Terraneo, G., Barrett, C. J., Resnati, G., Metrangolo, P. & Primägi, A., 28 Jan 2015, In : Journal of Materials Chemistry C. 3, p. 759-768 10 p.

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

#### **Silver sulfide nanoclusters and the superatom model**

Goh, J-Q., Malola, S., Häkkinen, H. & Akola, J., 22 Jan 2015, In : Journal of Physical Chemistry C. 119, 3, p. 1583-1590 8 p.

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

#### **Kinetics of polymer looping with macromolecular crowding: Effects of volume fraction and crowder size**

Shin, J., Cherstvy, A. G. & Metzler, R., 21 Jan 2015, In : Soft Matter. 11, 3, p. 472-488 17 p.

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

#### **Non-universal tracer diffusion in crowded media of non-inert obstacles**

Ghosh, S. K., Cherstvy, A. G. & Metzler, R., 21 Jan 2015, In : Physical Chemistry Chemical Physics. 17, 3, p. 1847-1858 12 p.

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

#### **Rational design of a printable, highly conductive silicone-based electrically conductive adhesive for stretchable radio-frequency antennas**

Li, Z., Le, T., Wu, Z., Yao, Y., Li, L., Tentzeris, M., Moon, K. S. & Wong, C. P., 21 Jan 2015, In : Advanced Functional Materials. 25, 3, p. 464-470 7 p.

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

#### **Second-Harmonic Generation from Metal Nanoparticles: Resonance Enhancement versus Particle Geometry**

Czaplicki, R., Mäkitalo, J., Siikanen, R., Husu, H., Lehtolahti, J., Kuittinen, M. & Kauranen, M., 14 Jan 2015, In : Nano Letters. 15, 1, p. 530-534 5 p.

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

#### **Oxidation half-reaction of aqueous nucleosides and nucleotides via photoelectron spectroscopy augmented by ab initio calculations**

Schroeder, C. A., Pluharová, E., Seidel, R., Schroeder, W. P., Faubel, M., Slavíček, P., Winter, B., Jungwirth, P. & Bradforth, S. E., 14 Jan 2015, In : Journal of the American Chemical Society. 137, 1, p. 201-209 9 p.

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

#### **Manipulation of polycarbonate urethane bulk properties via incorporated zwitterionic polynorborene for tissue engineering application**

Khan, M., Yang, J., Shi, C., Feng, Y., Zhang, W., Gibney, K. & Tew, G. N., 6 Jan 2015, In : RSC Advances. 5, 15, p. 11284-11292

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

#### **Photophysical properties of Sn (IV)tetraphenylporphyrin-pyrene dyad with a $\beta$ -vinyl linker**

Reeta, P. S., Khetubol, A., Jella, T., Chukharev, V., Abou-Chahine, F., Tkachenko, N. V., Giribabu, L. & Lemmetyinen, H., 1 Jan 2015, In : Journal of Porphyrins and Phthalocyanines. 19, 1-3, p. 288-300 13 p.

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

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

Yi, H., Albrecht, M., Valkonen, A. & Rissanen, K., 1 Jan 2015, In : New Journal of Chemistry. 39, 1, p. 746-749 4 p.

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

**A comparison of five optical surface topography measurement methods**

Mettänen, M. & Hirn, U., 1 Jan 2015, In : TAPPI Journal. 14, 1, p. 27-38 12 p.

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

**Appropriate pricing policy needed worldwide for improving water services infrastructure**

Hukka, J. J. & Katko, T. S., 1 Jan 2015, In : Journal American Water Works Association. 107, 1, p. E37-E46

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

**$\pi$ -Expanded  $\alpha,\beta$ -unsaturated ketones: Synthesis, optical properties, and two-photon-induced polymerization**

Nazir, R., Bourquard, F., Balčiūnas, E., Smoleń, S., Gray, D., Tkachenko, N. V., Farsari, M. & Gryko, D. T., 2015, In : ChemPhysChem. 16, 3, p. 682–690 9 p.

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

**Role of the bridge in photoinduced electron transfer in porphyrin-fullerene dyads**

Pelado, B., Abou-Chahine, F., Calbo, J., Caballero, R., delaCruz, P., Junquera-Hernández, J. M., Ortí, E., Tkachenko, N. V. & Langa, F., 2015, In : Chemistry: A European Journal. 21, 15, p. 5814-5825 12 p.

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

**Ballistic and numerical simulation of impacting goods on conveyor belt rubber**

Molnar, W., Nugent, S., Lindroos, M., Apostol, M. & Varga, M., 2015, In : Polymer Testing. 42, p. 1-7 7 p.

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

**Synthesis of fluorescent naphthoquinolizines via intramolecular houben-hoesch reaction**

Stasyuk, A. J., Smoleń, S., Glodkowska-Mrowka, E., Brutkowski, W., Cyrański, M. K., Tkachenko, N. & Gryko, D. T., 2015, In : Chemistry - An Asian Journal. 10, 3, p. 553-558 6 p.

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**

Wacharine, I., Valkonen, A., Rzaigui, M. & Smirani, W., 2015, In : Monatshefte fur Chemie. 146, 12, p. 2007-2020 14 p.

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

**Chemolithotrophic denitrification in biofilm reactors**

Di Capua, F., Papirio, S., Lens, P. N. L. & Esposito, G., 2015, In : Chemical Engineering Journal. 280, p. 643-657 15 p.

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

**Van der Waals interactions are critical in Car-Parrinello molecular dynamics simulations of porphyrin-fullerene dyads**

Karilainen, T., Cramariuc, O., Kuisma, M., Tappura, K. & Hukka, T. I., 2015, In : Journal of Computational Chemistry. 36, 9, p. 612-621 10 p.

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

**Characterisation of novel regenerated cellulosic, viscose, and cotton fibres and the dyeing properties of fabrics**

Kamppuri, T., Vehviläinen, M., Puolakka, A., Honkanen, M., Vippola, M. & Rissanen, M., 2015, In : Coloration Technology. 131, 5, p. 396-402 7 p.

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

**Geometry controlled anomalous diffusion in random fractal geometries: Looking beyond the infinite cluster**

Mardoukhi, Y., Jeon, J-H. & Metzler, R., 2015, In : Physical Chemistry Chemical Physics. 17, 44, p. 30134-30147 14 p.

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

**Stimuli-Responsive Materials Based on Interpenetrating Polymer Liquid Crystal Hydrogels**

Stumpel, J. E., Gil, E. R., Spoelstra, A. B., Bastiaansen, C. W. M., Broer, D. J. & Schenning, A. P. H. J., 2015, In : Advanced Functional Materials. 25, 22, p. 3314–3320

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

**Water-responsive dual-coloured photonic polymer coatings based on cholesteric liquid crystals**

Stumpel, J. E., Broer, D. J. & Schenning, A. P. H. J., 2015, In : RSC Advances. 5, 115, p. 94650-94653 4 p.

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

**Coulomb explosion during the early stages of the reaction of alkali metals with water**

Mason, P. E., Uhlig, F., Vaněk, V., Buttersack, T., Bauerecker, S. & Jungwirth, P., 2015, In : Nature Chemistry. 7, 3, p. 250-254 5 p.

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

**Block co-polymers for nanolithography: Rapid microwave annealing for pattern formation on substrates**

Borah, D., Rasappa, S., Sentharamaiah, R., Holmes, J. D. & Morris, M. A., 2015, In : Polymers. 7, 4, p. 592-609 18 p.

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

**Switchavidin: Reversible biotin-avidin-biotin bridges with high affinity and specificity**

Taskinen, B., Zauner, D., Lehtonen, S. I., Koskinen, M., Thomson, C., Kähkönen, N., Kukkurainen, S., Määttä, J. A. E., Ihalainen, T. O., Kulomaa, M. S., Gruber, H. J. & Hytönen, V. P., 17 Dec 2014, In : Bioconjugate Chemistry. 25, 12, p. 2233-2243 11 p.

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

**DNA lesion can facilitate base ionization: Vertical ionization energies of aqueous 8-oxoguanine and its nucleoside and nucleotide**

Palivec, V., Pluharová, E., Unger, I., Winter, B. & Jungwirth, P., 4 Dec 2014, In : Journal of Physical Chemistry Part B. 118, 48, p. 13833-13837 5 p.

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

**Time-resolved fluorescence methods (IUPAC technical report)**

Lemmetyinen, H., Tkachenko, N. V., Valeur, B., Hotta, J. I., Ameloot, M., Ernsting, N. P., Gustavsson, T. & Boens, N., 1 Dec 2014, In : Pure and Applied Chemistry. 86, 12, p. 1969-1998 30 p.

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

**Processable aromatic polyesters based on bisphenol derived from cashew nut shell liquid: synthesis and characterization**

Tawade, B. V., Salunke, J. K., Sane, P. S. & Wadgaonkar, P. P., 18 Nov 2014, In : JOURNAL OF POLYMER RESEARCH. 21, 12

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

**Electromagnetic interference shielding effectiveness of MWCNT filled poly(ether sulfone) and poly(ether imide) nanocomposites**

Mohanty, A. K., Ghosh, A., Sawai, P., Pareek, K., Banerjee, S., Das, A., Pötschke, P., Heinrich, G. & Voit, B., 1 Nov 2014, In : Polymer Engineering and Science. 54, 11, p. 2560-2570 11 p.

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

**A supramolecular approach to photoresponsive thermo/solvoplastic block copolymer elastomers**

Wang, X., Vapaavuori, J., Zhao, Y. & Bazuin, C. G., 28 Oct 2014, In : Macromolecules. 47, 20, p. 7099-7108 10 p.

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

**Impact of selective catalytic reduction on exhaust particle formation over excess ammonia events**

Amanatidis, S., Ntziachristos, L., Giechaskiel, B., Bergmann, A. & Samaras, Z., 7 Oct 2014, In : Environmental Science and Technology. 48, 19, p. 11527-11534 8 p.

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

**Global analysis of human nonreceptor tyrosine kinase specificity using high-density peptide microarrays**

Deng, Y., Alicea-Velázquez, N. L., Bannwarth, L., Lehtonen, S. I., Boggon, T. J., Cheng, H. C., Hytönen, V. P. & Turk, B. E., 3 Oct 2014, In : Journal of Proteome Research. 13, 10, p. 4339-4346 8 p.

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

### **Rapid, Brushless Self-assembly of a PS-b-PDMS Block Copolymer for Nanolithography**

Rasappa, S., Schulte, L., Borah, D., Morris, M. A. & Ndoni, S., 1 Oct 2014, In : Colloids and Interface Science Communications. 2, p. 1-5 5 p.

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

### **Effect of head group size on the photoswitching applications of azobenzene Disperse Red 1 analogues**

Goulet-Hanssens, A., Corkery, T. C., Priimagi, A. & Barrett, C. J., 28 Sep 2014, In : Journal of Materials Chemistry C. 2, 36, p. 7505-7512 8 p.

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

### **Pyrene based conjugated materials: Synthesis, characterization and electroluminescent properties**

Salunke, J. K., Sonar, P., Wong, F. L., Roy, V. A. L., Lee, C. S. & Wadgaonkar, P. P., 26 Sep 2014, In : Physical Chemistry Chemical Physics. 16, 42, p. 23320-23328 9 p.

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

### **Density functional theory study of transition metals doped B<sub>80</sub> fullerene**

Wang, J., Ma, L., Liang, Y., Gao, M. & Wang, G., 22 Sep 2014, In : Journal of Theoretical and Computational Chemistry. 13, 6, 1450050.

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

### **Recent twists in photoactuation and photoalignment control**

Priimagi, A., Barrett, C. J. & Shishido, A., 21 Sep 2014, In : Journal of Materials Chemistry C. 2, 35, p. 7155-7162 8 p.

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

### **Optical spectroscopy of the bulk and interfacial hydrated electron from ab initio calculations**

Uhlig, F., Herbert, J. M., Coons, M. P. & Jungwirth, P., 4 Sep 2014, In : Journal of Physical Chemistry A. 118, 35, p. 7507-7515 9 p.

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

### **The role of linked phospholipids in the rubber-filler interaction in carbon nanotube (CNT) filled natural rubber (NR) composites**

Le, H. H., Abhijeet, S., Ilisch, S., Klehm, J., Henning, S., Beiner, M., Sarkawi, S. S., Dierkes, W., Das, A., Fischer, D., Stöckelhuber, K. W., Wiessner, S., Khatiwada, S. P., Adhikari, R., Pham, T., Heinrich, G. & Radsch, H. J., 2 Sep 2014, In : Polymer. 55, 18, p. 4738-4747 10 p.

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

### **Effect of silane integrated sol-gel derived in situ silica on the properties of nitrile rubber**

Kapgate, B. P., Das, C., Basu, D., Das, A., Heinrich, G. & Reuter, U., 5 Aug 2014, In : Journal of Applied Polymer Science. 131, 15, 40531.

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

### **Molecular engineering of avidin and hydrophobin for functional self-assembling interfaces**

Kurppa, K., Hytönen, V. P., Nakari-Setälä, T., Kulomaa, M. S. & Linder, M. B., 1 Aug 2014, In : Colloids and Surfaces B: Biointerfaces. 120, p. 102-109 8 p.

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

### **Performance testing of iron based thermally sprayed HVOF coatings in a biomass-fired fluidised bed boiler**

Oksa, M., Varis, T. & Ruusuvoori, K., 25 Jul 2014, In : Surface and Coatings Technology. 251, p. 191-200 10 p.

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

### **Accurate description of calcium solvation in concentrated aqueous solutions**

Kohagen, M., Mason, P. E. & Jungwirth, P., 17 Jul 2014, In : Journal of Physical Chemistry Part B. 118, 28, p. 7902-7909 8 p.

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

**Surface behavior of hydrated guanidinium and ammonium ions: A comparative study by photoelectron spectroscopy and molecular dynamics**

Werner, J., Wernersson, E., Ekholm, V., Ottosson, N., Öhrwall, G., Heyda, J., Persson, I., Söderström, J., Jungwirth, P. & Björneholm, O., 26 Jun 2014, In : Journal of Physical Chemistry Part B. 118, 25, p. 7119-7127 9 p.

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

**Carbon nanotubes-filled thermoplastic polyurethane-urea and carboxylated acrylonitrile butadiene rubber blend nanocomposites**

Mahmood, N., Khan, A. U., Stöckelhuber, K. W., Das, A., Jehnichen, D. & Heinrich, G., 5 Jun 2014, In : Journal of Applied Polymer Science. 131, 11

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

**Hydration of the chloride ion in concentrated aqueous solutions using neutron scattering and molecular dynamics**

Pluhařová, E., Fischer, H. E., Mason, P. E. & Jungwirth, P., 19 May 2014, In : Molecular Physics. 112, 9-10, p. 1230-1240 11 p.

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

**Bioprocessing of enhanced cellulase production from a mutant of Trichoderma asperellum RCK2011 and its application in hydrolysis of cellulose**

Raghuwanshi, S., Deswal, D., Karp, M. & Kuhad, R. C., 15 May 2014, In : Fuel. 124, p. 183-189 7 p.

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

**Light-fuelled transport of large dendrimers and proteins**

Koskela, J. E., Liljeström, V., Lim, J., Simanek, E. E., Ras, R. H. A., Priimagi, A. & Kostianen, M. A., 14 May 2014, In : Journal of the American Chemical Society. 136, 19, p. 6850-6853 4 p.

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

**Microphase mechanism of "superquenching" of luminescent probes in aqueous solutions of DNA and some other polyelectrolytes**

Kuzmin, M. G., Soboleva, I. V., Durandin, N. A., Lisitsyna, E. S. & Kuzmin, V. A., 17 Apr 2014, In : Journal of Physical Chemistry Part B. 118, 15, p. 4245-4252 8 p.

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

**Protein conformation as a regulator of cell-matrix adhesion**

Hytönen, V. P. & Wehrle-Haller, B., 14 Apr 2014, In : Physical Chemistry Chemical Physics. 16, 14, p. 6342-6357 16 p.

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

**Deciphering the infrared spectrum of the protonated water pentamer and the hybrid Eigen-Zundel cation**

Kulig, W. & Agmon, N., 14 Mar 2014, In : Physical Chemistry Chemical Physics. 16, 10, p. 4933-4941 9 p.

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

**Fabrication of ssDNA/oligo(ethylene glycol) monolayers by promoted exchange reaction with thiol and disulfide substituents**

Khan, M. N. & Zharnikov, M., 13 Feb 2014, In : Journal of Physical Chemistry C. 118, 6, p. 3093-3101 9 p.

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

**Azopolymer-based micro- and nanopatterning for photonic applications**

Priimagi, A. & Shevchenko, A., 1 Feb 2014, In : Journal of Polymer Science. Part B, Polymer Physics. 52, 3, p. 163-182 20 p.

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

**Both zundel and eigen isomers contribute to the IR spectrum of the gas-phase H<sub>9</sub>O<sub>4</sub><sup>+</sup> cluster**

Kulig, W. & Agmon, N., 9 Jan 2014, In : Journal of Physical Chemistry Part B. 118, 1, p. 278-286 9 p.

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

**Natural thermal adaptation increases heat shock protein levels and decreases oxidative stress**

Oksala, N. K. J., Ekmekçi, F. G., Özsoy, E., Kirankaya, Ş., Kokkola, T., Emecen, G., Lappalainen, J., Kaarniranta, K. & Atalay, M., 1 Jan 2014, In : REDOX BIOLOGY. 3, p. 25-28 4 p.

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

**A microscopic view of the mechanisms of active transport across the cellular membrane**

Enkavi, G., Li, J., Wen, P., Thangapandian, S., Moradi, M., Jiang, T., Han, W. & Tajkhorshid, E., 2014, In : Annual Reports in Computational Chemistry. 10, p. 77-125 49 p.

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

**Direct observation of the collapse of the delocalized excess electron in water**

Savolainen, J., Uhlig, F., Ahmed, S., Hamm, P. & Jungwirth, P., 2014, In : Nature Chemistry. 6, 8, p. 697-701 5 p.

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

**A full-potential linearized augmented plane wave study of the interaction of CO<sub>2</sub> with  $\alpha$ -Pu (020) surface nanolayers**

Wang, J. & Ray, A. K., 2014, In : Journal of Computational and Theoretical Nanoscience. 11, 7, p. 1710-1717 8 p.

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

**Molekuly a ionty v pohybu: Počítačové simulace biochemických a biofyzikálních procesů**

Jungwirth, P., 2014, In : Chemické Listy. 108, 4, p. 278-284 7 p.

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

**Magnetic origin of the chemical balance in alloyed Fe-Cr stainless steels: First-principles and Ising model study**

Airiskallio, E., Nurmi, E., Väyrynen, I. J., Kokko, K., Ropo, M., Punkkinen, M. P. J., Johansson, B. & Vitos, L., 2014, In : Computational Materials Science. 92, p. 135-140 6 p.

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

**Effect of non-rubber components of NR on the carbon nanotube (CNT) localization in SBR/NR blends**

Le, H. H., Parsekar, M., Ilisch, S., Henning, S., Das, A., Stöckelhuber, K. W., Beiner, M., Ho, C. A., Adhikari, R., Wießner, S., Heinrich, G. & Radusch, H. J., 2014, In : Macromolecular Materials and Engineering. 299, 5, p. 569-582 14 p.

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

**Novel derivatives of bacteriochlorophyll a: Complex formation with albumin and the mechanism of tumor cell photodamage**

Akimova, A. V., Grin, M. A., Golovina, G. V., Kokrashvili, T. A., Vinogradov, A. M., Mironov, A. F., Rychkov, G. N., Shtil, A. A., Kuzmin, V. A. & Durandin, N. A., 2014, In : DOKLADY BIOCHEMISTRY AND BIOPHYSICS. 454, 1, p. 17-20 4 p.

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

**Fabrication of 3-D nanodimensioned electric double layer capacitor structures using block copolymer templates**

Rasappa, S., Borah, D., Senthamaraiannan, R., Faulkner, C. C., Holmes, J. D. & Morris, M. A., 2014, In : Journal Nanoscience and Nanotechnology. 14, 7, p. 5221-5227 7 p.

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

**Study of the kinetics and mechanism of rapid self-assembly in block copolymer thin films during solvo-microwave annealing**

Mokarian-Tabari, P., Cummins, C., Rasappa, S., Simao, C., Torres, C. M. S., Holmes, J. D. & Morris, M. A., 2014, In : Langmuir. 30, 35, p. 10728-10739 12 p.

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

**Kinetics of bioconjugate nanoparticle label binding in a sandwich-type immunoassay**

Näreoja, T., Ebner, A., Gruber, H. J., Taskinen, B., Kienberger, F., Hänninen, P. E., Hytönen, V. P., Hinterdorfer, P. & Härmä, H., 2014, In : Analytical and Bioanalytical Chemistry. 406, 2, p. 493-503 11 p.

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

**Self-assembly of polystyrene-block-poly(4-vinylpyridine) block copolymer on molecularly functionalized silicon substrates: Fabrication of inorganic nanostructured etchmask for lithographic use**

Cummins, C., Borah, D., Rasappa, S., Chaudhari, A., Ghoshal, T., O'Driscoll, B. M. D., Carolan, P., Petkov, N., Holmes, J. D. & Morris, M. A., 21 Dec 2013, In : *Journal of Materials Chemistry C*. 1, 47, p. 7941-7951 11 p.

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

**Analysis of free, mono- and diacetylated polyamines from human urine by LC-MS/MS**

Häkkinen, M. R., Roine, A., Auriola, S., Tuokko, A., Veskimäe, E., Keinänen, T. A., Lehtimäki, T., Oksala, N. & Vepsäläinen, J., 15 Dec 2013, In : *JOURNAL OF CHROMATOGRAPHY B: ANALYTICAL TECHNOLOGIES IN THE BIOMEDICAL AND LIFE SCIENCES*. 941, p. 81-89 9 p.

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

**Location of dispersing agent in rubber nanocomposites during mixing process**

Le, H. H., Oßwald, K., Wießner, S., Das, A., Stöckelhuber, K. W., Boldt, R., Gupta, G., Heinrich, G. & Radusch, H. J., 13 Dec 2013, In : *Polymer*. 54, 26, p. 7009-7021 13 p.

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

**Proliferation and differentiation of adipose stem cells towards smooth muscle cells on poly(trimethylene carbonate) membranes**

German, S. J., Behbahani, M., Miettinen, S., Grijpma, D. W. & Haimi, S. P., Dec 2013, In : *Macromolecular symposia*. 334, 1, p. 133-142 10 p.

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

**Effect of surface morphology of poly( $\epsilon$ -caprolactone) scaffolds on adipose stem cell adhesion and proliferation**

Diban, N., Haimi, S. P., Bolhuis-Versteeg, L., Teixeira, S., Miettinen, S., Poot, A. A., Grijpma, D. W. & Stamatialis, D., Dec 2013, In : *Macromolecular symposia*. 334, 1, p. 126-132 7 p.

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

**Human adipose stem cells in chondrogenic differentiation medium without growth factors differentiate towards annulus fibrosus phenotype in vitro**

Gebraad, A. W. H., Miettinen, S., Grijpma, D. W. & Haimi, S. P., Dec 2013, In : *Macromolecular symposia*. 334, 1, p. 49-56 8 p.

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

**Fabrication of ssDNA/Oligo(ethylene glycol) monolayers and patterns by exchange reaction promoted by ultraviolet light irradiation**

Khan, M. N. & Zharnikov, M., 27 Nov 2013, In : *Journal of Physical Chemistry C*. 117, 47, p. 24883-24893 11 p.

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

**Release of halide ions from the buried active site of the haloalkane dehalogenase LinB revealed by stopped-flow fluorescence analysis and free energy calculations**

Hladilkova, J., Prokop, Z., Chaloupkova, R., Damborsky, J. & Jungwirth, P., 21 Nov 2013, In : *Journal of Physical Chemistry Part B*. 117, 46, p. 14329-14335 7 p.

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

**Ion pairing in aqueous lithium salt solutions with monovalent and divalent counter-anions**

Pluhařová, E., Mason, P. E. & Jungwirth, P., 21 Nov 2013, In : *Journal of Physical Chemistry A*. 117, 46, p. 11766-11773 8 p.

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

**The Halogen Bond in the Design of Functional Supramolecular Materials: Recent Advances**

Primagi, A., Cavallo, G., Metrangolo, P. & Resnati, G., 19 Nov 2013, In : *Accounts of Chemical Research*. 46, 11, p. 2686-2695 10 p.

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

**How conformational flexibility stabilizes the hyperthermophilic elongation factor G-domain**

Kalimeri, M., Rahaman, O., Melchionna, S. & Sterpone, F., 7 Nov 2013, In : *Journal of Physical Chemistry Part B*. 117, 44, p. 13775-13785 11 p.

#### **Embedded cluster models for reactivity of the hydrated electron**

Uhlig, F. & Jungwirth, P., Nov 2013, In : ZEITSCHRIFT FUR PHYSIKALISCHE CHEMIE-INTERNATIONAL JOURNAL OF RESEARCH IN PHYSICAL CHEMISTRY AND CHEMICAL PHYSICS. 227, 11, p. 1583-1593 11 p.

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

#### **Soft-graphoepitaxy using nanoimprinted polyhedral oligomeric silsesquioxane substrates for the directed self-Assembly of PS-b-PDMS**

Borah, D., Simao, C. D., Senthamaraiannan, R., Rasappa, S., Francone, A., Lorret, O., Salaun, M., Kosmala, B., Kehagias, N., Zelsmann, M., Sotomayor-Torres, C. M. & Morris, M. A., Nov 2013, In : European Polymer Journal. 49, 11, p. 3512-3521 10 p.

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

#### **Porphyrin adsorbed on the (1010) surface of the wurtzite structure of ZnO-conformation induced effects on the electron transfer characteristics**

Niskanen, M., Kuisma, M., Cramariuc, O., Golovanov, V., Hukka, T. I., Tkachenko, N. & Rantala, T. T., 28 Oct 2013, In : Physical Chemistry Chemical Physics. 15, 40, p. 17408-17418 11 p.

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

#### **Reversible biofunctionalization of surfaces with a switchable mutant of avidin**

Pollheimer, P., Taskinen, B., Scherfler, A., Gusenkov, S., Creus, M., Wiesauer, P., Zauner, D., Schöfberger, W., Schwarzinger, C., Ebner, A., Tampé, R., Stutz, H., Hytönen, V. P. & Gruber, H. J., 16 Oct 2013, In : Bioconjugate Chemistry. 24, 10, p. 1656-1668 13 p.

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

#### **Importance of the ion-pair interactions in the OPEP coarse-grained force field: Parametrization and validation**

Sterpone, F., Nguyen, P. H., Kalimeri, M. & Derreumaux, P., 8 Oct 2013, In : Journal of Chemical Theory and Computation. 9, 10, p. 4574-4584 11 p.

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

#### **Zinc coordination spheres in protein structures**

Laitaoja, M., Valjakka, J. & Jänis, J., 7 Oct 2013, In : Inorganic Chemistry. 52, 19, p. 10983-10991 9 p.

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

#### **Spectroscopic study of a DNA brush synthesized in situ by surface initiated enzymatic polymerization**

Khan, M. N., Tjong, V., Chilkoti, A. & Zharnikov, M., 29 Aug 2013, In : Journal of Physical Chemistry Part B. 117, 34, p. 9929-9938 10 p.

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

#### **Mechanisms of acceleration and retardation of water dynamics by ions**

Stirnemann, G., Wernersson, E., Jungwirth, P. & Laage, D., 14 Aug 2013, In : Journal of the American Chemical Society. 135, 32, p. 11824-11831 8 p.

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

#### **Irradiation promoted exchange reaction with disulfide substituents**

Khan, M. N. & Zharnikov, M., 18 Jul 2013, In : Journal of Physical Chemistry C. 117, 28, p. 14534-14543 10 p.

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

#### **Tuning PDMS brush chemistry by UV-O3 exposure for PS-b-PDMS microphase separation and directed self-assembly**

Borah, D., Rasappa, S., Senthamaraiannan, R., Holmes, J. D. & Morris, M. A., 16 Jul 2013, In : Langmuir. 29, 28, p. 8959-8968 10 p.

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

#### **Reversal of the hofmeister series: Specific ion effects on peptides**

Paterová, J., Rembert, K. B., Heyda, J., Kurra, Y., Okur, H. I., Liu, W. R., Hilty, C., Cremer, P. S. & Jungwirth, P., 11 Jul 2013, In : Journal of Physical Chemistry Part B. 117, 27, p. 8150-8158 9 p.



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

**Photoswitchable hydrogel surface topographies by polymerisation-induced diffusion**

Stumpel, J. E., Liu, D., Broer, D. J. & Schenning, A. P. H. J., 2 Jul 2013, In : *Chemistry: A European Journal*. 19, 33, p. 10922-10927 6 p.

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

**Development and characterization of poly( $\epsilon$ -caprolactone) hollow fiber membranes for vascular tissue engineering**

Diban, N., Haimi, S., Bolhuis-Versteeg, L., Teixeira, S., Miettinen, S., Poot, A., Grijpma, D. & Stamatialis, D., 1 Jul 2013, In : *Journal of Membrane Science*. 438, p. 29-37 9 p.

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

**Shape-dependent plasmonic response and directed self-assembly in a new semiconductor building block, indium-doped cadmium oxide (ICO)**

Gordon, T. R., Paik, T., Klein, D. R., Naik, G. V., Caglayan, H., Boltasseva, A. & Murray, C. B., 12 Jun 2013, In : *Nano Letters*. 13, 6, p. 2857-2863 7 p.

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

**Cell toxicity and oxidative potential of engine exhaust particles: Impact of using particulate filter or biodiesel fuel blend**

Gerlofs-Nijland, M. E., Totlandsdal, A. I., Tzankiozis, T., Leseman, D. L. A. C., Samaras, Z., Låg, M., Schwarze, P., Ntziachristos, L. & Cassee, F. R., 4 Jun 2013, In : *Environmental Science and Technology*. 47, 11, p. 5931-5938 8 p.

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

**Cation-specific effects on enzymatic catalysis driven by interactions at the tunnel mouth**

Štěpánková, V., Paterová, J., Damborský, J., Jungwirth, P., Chaloupková, R. & Heyda, J., 30 May 2013, In : *Journal of Physical Chemistry Part B*. 117, 21, p. 6394-6402 9 p.

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

**Surface properties and interaction forces of biopolymer-doped conductive polypyrrole surfaces by atomic force microscopy**

Pelto, J. M., Haimi, S. P., Siljander, A. S., Miettinen, S. S., Tappura, K. M., Higgins, M. J. & Wallace, G. G., 21 May 2013, In : *Langmuir*. 29, 20, p. 6099-6108 10 p.

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

**Depth profiling of PLGA copolymer in a novel biomedical bilayer using confocal raman spectroscopy**

McManamon, C., Delaney, P., Kavanagh, C., Wang, J. J., Rasappa, S. & Morris, M. A., 14 May 2013, In : *Langmuir*. 29, 19, p. 5905-5910 6 p.

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

**Screening pretreatment methods to enhance thermophilic anaerobic digestion of pulp and paper mill wastewater treatment secondary sludge**

Bayr, S., Kaparaju, P. & Rintala, J., 1 May 2013, In : *Chemical Engineering Journal*. 223, p. 479-486 8 p.

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

**Immobilized bioactive agents onto polyurethane surface with heparin and phosphorylcholine group**

Tan, M., Feng, Y., Wang, H., Zhang, L., Khan, M., Guo, J., Chen, Q. & Liu, J., May 2013, In : *Macromolecular Research*. 21, 5, p. 541-549 9 p.

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

**Nanoindentation study of light-induced softening of supramolecular and covalently functionalized azo polymers**

Vapaavuori, J., Mahimwalla, Z., Chromik, R. R., Kaivola, M., Priimagi, A. & Barrett, C. J., 28 Apr 2013, In : *Journal of Materials Chemistry C*. 1, 16, p. 2806-2810 5 p.

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

**Understanding the reinforcing behavior of expanded clay particles in natural rubber compounds**

Roop, S., Das, A., Stöckelhuber, K. W., Wang, D. Y., Galiatsatos, V. & Heinrich, G., 14 Apr 2013, In : *Soft Matter*. 9, 14, p. 3798-3808 11 p.

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

**Biomimetic zinc chlorin-poly(4-vinylpyridine) assemblies: Doping level dependent emission-absorption regimes**

Pale, V., Nikkonen, T., Vapaavuori, J., Kostiainen, M., Kavakka, J., Selin, J., Tittonen, I. & Helaja, J., 21 Mar 2013, In : Journal of Materials Chemistry C. 1, 11, p. 2166-2173 8 p.

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

**Site-specific analysis of dipole polarizabilities of heterogeneous systems: Iron-doped Si<sub>n</sub> (n = 1-14) clusters**

Ma, L., Wang, J. & Wang, G., 7 Mar 2013, In : Journal of Chemical Physics. 138, 9, 094304.

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

**Molecularly functionalized silicon substrates for orientation control of the microphase separation of PS-b-PMMA and PS-b-PDMS block copolymer systems**

Borah, D., Ozmen, M., Rasappa, S., Shaw, M. T., Holmes, J. D. & Morris, M. A., 5 Mar 2013, In : Langmuir. 29, 9, p. 2809-2820 12 p.

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

**Optical vortex generation in nematic liquid crystal light valves**

Barboza, R., Bortolozzo, U., Assanto, G. & Residori, S., 1 Mar 2013, In : Molecular Crystals and Liquid Crystals. 572, 1, p. 24-30 7 p.

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

**Fabrication of a sub-10 nm silicon nanowire based ethanol sensor using block copolymer lithography**

Rasappa, S., Borah, D., Faulkner, C. C., Lutz, T., Shaw, M. T., Holmes, J. D. & Morris, M. A., 15 Feb 2013, In : Nanotechnology. 24, 6, 065503.

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

**Aqueous guanidinium-carbonate interactions by molecular dynamics and neutron scattering: Relevance to ion-protein interactions**

Vazdar, M., Jungwirth, P. & Mason, P. E., 14 Feb 2013, In : Journal of Physical Chemistry Part B. 117, 6, p. 1844-1848 5 p.

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

**Chemically tailored dielectric-to-metal transition for the design of metamaterials from nanoimprinted colloidal nanocrystals**

Fafarman, A. T., Hong, S. H., Caglayan, H., Ye, X., Diroll, B. T., Paik, T., Engheta, N., Murray, C. B. & Kagan, C. R., 13 Feb 2013, In : Nano Letters. 13, 2, p. 350-357 8 p.

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

**Growth behavior and magnetic properties of spherical uranium oxide nanoclusters**

Ma, L. & Ray, A. K., Feb 2013, In : Journal of Computational and Theoretical Nanoscience. 10, 2, p. 334-340 7 p.

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

**Density functional theory study of FePd<sub>n</sub> (n = 2-14) clusters and interactions with small molecules**

Ma, L., Wang, J., Hao, Y. & Wang, G., Feb 2013, In : Computational Materials Science. 68, p. 166-173 8 p.

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

**Networking of ionic liquid modified CNTs in SSBR**

Subramaniam, K., Das, A., Simon, F. & Heinrich, G., Feb 2013, In : European Polymer Journal. 49, 2, p. 345-352 8 p.

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

**A potential nonthrombogenic small-diameter vascular scaffold with polyurethane/poly(ethylene glycol) hybrid materials by electrospinning technique**

Wang, H., Feng, Y., Zhao, H., Fang, Z., Khan, M. & Guo, J., Feb 2013, In : Journal Nanoscience and Nanotechnology. 13, 2, p. 1578-1582 5 p.

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

**A 'clusters-in-liquid' method for calculating infrared spectra identifies the proton-transfer mode in acidic aqueous solutions**

Kulig, W. & Agmon, N., Jan 2013, In : Nature Chemistry. 5, 1, p. 29-35 7 p.

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

**Molecular mechanism of T-cell protein tyrosine phosphatase (TCPTP) activation by mitoxantrone**

Ylilauri, M., Mattila, E., Nurminen, E. M., Käpylä, J., Niinivehmas, S. P., Määttä, J. A., Pentikäinen, U., Ivaska, J. & Pentikäinen, O. T., 2013, In : Biochimica et biophysica acta: proteins and proteomics. 1834, 10, p. 1988-1997 10 p.

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

**New reports on anti-bacterial and anti-candidal activities of fatty acid methyl esters (FAME) obtained from *Scenedesmus bijugatus* var. *bicellularis* biomass**

Mubarakali, D., Praveenkumar, R., Shenbagavalli, T., Mari Nivetha, T., Parveez Ahamed, A., Al-Dhabi, N. A. & Thajuddin, N., 28 Nov 2012, In : RSC Advances. 2, 30, p. 11552-11556 5 p.

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

**Semiclassical hybrid approach to condensed phase molecular dynamics: Application to the  $I_2Kr_{17}$  cluster**

Buchholz, M., Goletz, C. M., Grossmann, F., Schmidt, B., Heyda, J. & Jungwirth, P., 26 Nov 2012, In : Journal of Physical Chemistry A. 116, 46, p. 11199-11210 12 p.

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

**Peptide salt bridge stability: From gas phase via microhydration to bulk water simulations**

Pluhařová, E., Marsalek, O., Schmidt, B. & Jungwirth, P., 14 Nov 2012, In : Journal of Chemical Physics. 137, 18, 185101.

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

**Search for global minimum geometries of medium sized  $Cd_nTe_n$  clusters ( $n = 15, 16, 20, 24$  and  $28$ )**

Ma, L., Wang, J. & Wang, G., 12 Nov 2012, In : Chemical Physics Letters. 552, p. 73-77 5 p.

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

**Transforming anion instability into stability: Contrasting photoionization of three protonation forms of the phosphate ion upon moving into water**

Pluhařová, E., Ončák, M., Seidel, R., Schroeder, C., Schroeder, W., Winter, B., Bradforth, S. E., Jungwirth, P. & Slaviček, P., 8 Nov 2012, In : Journal of Physical Chemistry Part B. 116, 44, p. 13254-13264 11 p.

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

**Influence of ionic liquids on the dielectric relaxation behavior of CNT based elastomer nanocomposites**

Steinhauser, D., Subramaniam, K., Das, A., Heinrich, G. & Klüppel, M., Nov 2012, In : Express Polymer Letters. 6, 11, p. 927-936 10 p.

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

**Azobenzene photomechanics: Prospects and potential applications**

Mahimwalla, Z., Yager, K. G., Mamiya, J. I., Shishido, A., Priimagi, A. & Barrett, C. J., Nov 2012, In : Polymer Bulletin. 69, 8, p. 967-1006 40 p.

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

**Superquenching of SYBRGreen dye fluorescence in complex with DNA by gold nanoparticles**

Lisitsyna, E. S., Lygo, O. N., Durandin, N. A., Dement'eva, O. V., Rudoi, V. M. & Kuzmin, V. A., Nov 2012, In : HIGH ENERGY CHEMISTRY. 46, 6, p. 363-367 5 p.

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

**Fabrication of ssDNA/oligo(ethylene glycol) monolayers and complex nanostructures by an irradiation-promoted exchange reaction**

Khan, M. N., Tjong, V., Chilkoti, A. & Zharnikov, M., 8 Oct 2012, In : Angewandte Chemie (International Edition). 51, 41, p. 10303-10306 4 p.

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

**Kinetics of filler wetting and dispersion in carbon nanotube/rubber composites**

Le, H. H., Hoang, X. T., Das, A., Gohs, U., Stoeckelhuber, K. W., Boldt, R., Heinrich, G., Adhikari, R. & Radusch, H. J., Oct 2012, In : Carbon. 50, 12, p. 4543-4556 14 p.

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

**Biomimetic surface modification of polycarbonateurethane film via phosphorylcholine-graft for resisting platelet adhesion**

Gao, W., Feng, Y., Lu, J., Khan, M. & Guo, J., Oct 2012, In : Macromolecular Research. 20, 10, p. 1063-1069 7 p.

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

**Affine-response model of molecular solvation of ions: Accurate predictions of asymmetric charging free energies**

Bardhan, J. P., Jungwirth, P. & Makowski, L., 28 Sep 2012, In : Journal of Chemical Physics. 137, 12, 124101.

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

**Effect of sol-gel derived in situ silica on the morphology and mechanical behavior of natural rubber and acrylonitrile butadiene rubber blends**

Kapgate, B. P., Das, C., Das, A., Basu, D., Reuter, U. & Heinrich, G., Sep 2012, In : JOURNAL OF SOL-GEL SCIENCE AND TECHNOLOGY. 63, 3, p. 501-509 9 p.

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

**Solvation and ion-pairing properties of the aqueous sulfate anion: Explicit versus effective electronic polarization**

Pegado, L., Marsalek, O., Jungwirth, P. & Wernersson, E., 7 Aug 2012, In : Physical Chemistry Chemical Physics. 14, 29, p. 10248-10257 10 p.

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

**Impact of biodiesel application at various blending ratios on passenger cars of different fueling technologies**

Kousoulidou, M., Ntziachristos, L., Fontaras, G., Martini, G., Dilara, P. & Samaras, Z., Aug 2012, In : Fuel. 98, p. 88-94 7 p.

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

**Accurate description of aqueous carbonate ions: An effective polarization model verified by neutron scattering**

Mason, P. E., Wernersson, E. & Jungwirth, P., 19 Jul 2012, In : Journal of Physical Chemistry Part B. 116, 28, p. 8145-8153 9 p.

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

**Nematicons in azobenzene liquid crystals**

Serak, S. V., Tabiryan, N. V. & Assanto, G., 19 Jul 2012, In : Molecular Crystals and Liquid Crystals. 559, p. 202-213 12 p.

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

**Molecular mechanisms of ion-specific effects on proteins**

Rembert, K. B., Paterová, J., Heyda, J., Hilty, C., Jungwirth, P. & Cremer, P. S., 20 Jun 2012, In : Journal of the American Chemical Society. 134, 24, p. 10039-10046 8 p.

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

**Halogen bonding versus hydrogen bonding in driving self-assembly and performance of light-responsive supramolecular polymers**

Priimagi, A., Cavallo, G., Forni, A., Gorynsztejn-Leben, M., Kaivola, M., Metrangolo, P., Milani, R., Shishido, A., Pilati, T., Resnati, G. & Terraneo, G., 20 Jun 2012, In : Advanced Functional Materials. 22, 12, p. 2572-2579 8 p.

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

**Behavior of 4-hydroxynonenal in phospholipid membranes**

Vazdar, M., Jurkiewicz, P., Hof, M., Jungwirth, P. & Cwiklik, L., 7 Jun 2012, In : Journal of Physical Chemistry Part B. 116, 22, p. 6411-6415 5 p.

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

#### **Elemental and mixed actinide dioxides: An ab initio study**

Ma, L., Atta-Fynn, R. & Ray, A. K., Jun 2012, In : Journal of Theoretical and Computational Chemistry. 11, 3, p. 611-629 19 p.

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

#### **Structural characteristics and flammability of fire retarding EPDM/layered double hydroxide (LDH) nanocomposites**

Wang, D. Y., Das, A., Leuteritz, A., Mahaling, R. N., Jehnichen, D., Wagenknecht, U. & Heinrich, G., 21 Apr 2012, In : RSC Advances. 2, 9, p. 3927-3933 7 p.

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

#### **Highly exfoliated natural rubber/Clay composites by "propping-open procedure": The influence of fatty-acid chain length on exfoliation**

Rooj, S., Das, A., Stöckelhuber, K. W., Reuter, U. & Heinrich, G., Apr 2012, In : Macromolecular Materials and Engineering. 297, 4, p. 369-383 15 p.

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

#### **Excited-state polarizability in crystalline sexithiophene: Charge-transfer and vibronic effects**

Stradomska, A., Kulig, W., Slawik, M. & Petelenz, P., 9 Mar 2012, In : Chemical Physics Letters. 529, p. 27-30 4 p.

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

#### **A novel thermotropic elastomer based on highly-filled LDH-SSB composites**

Das, A., George, J. J., Kutlu, B., Leuteritz, A., Wang, D. Y., Rooj, S., Jurk, R., Rajeshbabu, R., Stöckelhuber, K. W., Galiatsatos, V. & Heinrich, G., 27 Feb 2012, In : Macromolecular Rapid Communications. 33, 4, p. 337-342 6 p.

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

#### **Glycerol mediated synthesis of 5-substituted 1H-tetrazole under catalyst free conditions**

Nandre, K. P., Salunke, J. K., Nandre, J. P., Patil, V. S., Borse, A. U. & Bhosale, S. V., Feb 2012, In : Chinese Chemical Letters. 23, 2, p. 161-164 4 p.

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

#### **Surface-relief gratings and stable birefringence inscribed using light of broad spectral range in supramolecular polymer-bisazobenzene complexes**

Koskela, J. E., Vapaavuori, J., Hautala, J., Priimagi, A., Faul, C. F. J., Kaivola, M. & Ras, R. H. A., 26 Jan 2012, In : Journal of Physical Chemistry C. 116, 3, p. 2363-2370 8 p.

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

#### **Structure, dynamics, and reactivity of hydrated electrons by Ab initio molecular dynamics**

Marsalek, O., Uhlig, F., Vandevondele, J. & Jungwirth, P., 17 Jan 2012, In : Accounts of Chemical Research. 45, 1, p. 23-32 10 p.

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

#### **Layered Double Hydroxides (LDH): A multifunctional versatile system for nanocomposites**

Leuteritz, A., Kutlu, B., Meinel, J., Wang, D., Das, A., Wagenknecht, U. & Heinrich, G., 2012, In : Molecular Crystals and Liquid Crystals. 556, p. 107-113 7 p.

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

#### **Location of the Azobenzene moieties within the cross-linked liquid-crystalline polymers can dictate the direction of photoinduced bending**

Priimagi, A., Shimamura, A., Kondo, M., Hiraoka, T., Kubo, S., Mamiya, J. I., Kinoshita, M., Ikeda, T. & Shishido, A., 2012, In : ACS Macro Letters. 1, 1, p. 96-99 4 p.

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

#### **Chasing charge localization and chemical reactivity following photoionization in liquid water**

Marsalek, O., Elles, C. G., Pieniazek, P. A., Pluhaov, E., Vandevondele, J., Bradforth, S. E. & Jungwirth, P., 14 Dec 2011, In : Journal of Chemical Physics. 135, 22, 224510.

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

**The Discovery of Compounds That Stimulate the Activity of Kallikrein-Related Peptidase3 (KLK3)**

Härkönen, H. H., Mattsson, J. M., Määttä, J. A. E., Stenman, U. H., Koistinen, H., Matero, S., Windshügel, B., Poso, A. & Lahtela-Kakkonen, M., 9 Dec 2011, In : CHEMMEDCHEM. 6, 12, p. 2170-2178 9 p.

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

**Cholesterol driven alteration of the conformation and dynamics of phospholamban in model membranes**

Manna, M. & Mukhopadhyay, C., 7 Dec 2011, In : Physical Chemistry Chemical Physics. 13, 45, p. 20188-20198 11 p.

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

**Effect of ionic liquid on dielectric, mechanical and dynamic mechanical properties of multi-walled carbon nanotubes/polychloroprene rubber composites**

Subramaniam, K., Das, A., Steinhauser, D., Klüppel, M. & Heinrich, G., Dec 2011, In : European Polymer Journal. 47, 12, p. 2234-2243 10 p.

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

**Arrhenius analysis of anisotropic surface self-diffusion on the prismatic facet of ice**

Gładich, I., Pfalzgraff, W., Maršálek, O., Jungwirth, P., Roeselová, M. & Neshyba, S., 28 Nov 2011, In : Physical Chemistry Chemical Physics. 13, 44, p. 19960-19969 10 p.

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