In this work, we propose new field-free estimators of static field-gradient polarizabilities for finite temperature path-integral Monte Carlo method. Namely, dipole–quadrupole polarizability \( A \), dipole–dipole–quadrupole polarizability \( B \), and quadrupole–quadrupole polarizability \( C \) are computed for several up to two-electron systems: \( H, H^-, He, Li^+, Be^{2+}, Ps_2, PsH, H_2^+, H_2, H_3^+, \) and \( HeH^+ \). We provide complementary data for ground state electronic properties within the adiabatic approximation and demonstrate good agreement with available values in the literature. More importantly, we present fully non-adiabatic results from 50 K to 1600 K, which allow us to analyze and discuss strong thermal coupling and rovibrational effects in total field-gradient polarizabilities. These phenomena are most relevant but clearly overlooked, e.g., in the construction of modern polarizable force field models. However, our main purpose is demonstrating the accuracy and simplicity of our approach in a problem that is generally challenging.
investigate free atoms, molecules and clusters with photoelectron/photoion coincidence spectroscopy as well as solids with photoluminescence spectroscopy whereas the other one will be dedicated to ultra-high vacuum studies of surfaces and interphases, utilizing X-ray photoelectron spectroscopy and X-ray absorption spectroscopy. This paper focuses on the optical design of the beamline and general design concepts of the gasphase and solid-state end stations.

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Scopus rating (2002): SJR 0.628 SNIP 1.108
Scopus rating (2001): SJR 0.688 SNIP 1.104
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Computing thermal effects on nonlinear optical properties of small atoms
The significance of nonlinear optical properties (NOP) is pronounced in many physical scales starting from microscopic interactions, such as van der Waals, to macroscopic properties, like dielectric constant and refractive index. Obtaining NOP, that is, dipole and multipole moments and (hyper)polarizabilities of matter, by computational simulation is particularly important in systems beyond experimental reach, such as exotic light-nucleus molecules in warm dense matter present in stars and gas planets, or short life-time particles such as positron. Most first-principles approaches are straightforward in 0
K but become tedious in thermal ensembles and beyond the adiabatic approximation.

The path-integral Monte Carlo method (PIMC) provides a tangible interface between the tensorial and the thermally averaged character of molecular (hyper)polarizabilities. In a recent study [1], we have derived field-free estimators that make the computation even more straightforward than our previous finite-field approach [2]. With the adiabatic, i.e. Born–Oppenheimer, approximation we obtain accurate tensorial ground state (hyper)polarizabilities, while the non-adiabatic simulation adds in considerable rovibrational effects and thermal coupling. In case of several two-electron systems, our results at the 0 K limit are either novel or in excellent agreement with the literature (e.g., see Fig. 1). Besides these results, we are presenting the derivation and demonstration of yet unpublished estimators for dipole-quadrupole polarizabilities of small molecules.
UPS and DFT investigation of the electronic structure of gas-phase trimesic acid

Benzene-1,3,5-tricarboxylic acid (trimesic acid, TMA) molecules in gas-phase have been investigated by using valence band photoemission. The photoelectron spectrum in the binding energy region from 9 to 22 eV is interpreted based on the density functional theory calculations. The electronic configuration that makes contribution to each transition is demonstrated. Furthermore, electronic structure of TMA is compared with benzene and benzoic acid (BA) in order to demonstrate changes in molecular orbital energies induced by addition of carboxyl groups to benzene ring.

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Scopus rating (2011): SJR 1.06 SNIP 0.842 CiteScore 1.68
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Scopus rating (2004): SJR 0.754 SNIP 0.759
Scopus rating (2003): SJR 1.093 SNIP 0.8
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Scopus rating (2001): SJR 0.872 SNIP 0.785
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Temperature and quantum effects on hydrogen–metal cluster interaction

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Single-frequency 571nm VECSEL for photo-ionization of magnesium
We report the development of an intracavity-frequency-doubled vertical external-cavity surface-emitting laser (VECSEL) emitting at 571 nm for photoionization of magnesium. The laser employs a V-cavity geometry with a gain chip at the end of one cavity arm and a lithium triborate (LBO) crystal for second harmonic generation. The gain chip has a bottom-emitting design with ten GaInAs quantum wells of 7 nm thickness, which are strain compensated by GaAsP. The system is capable of producing up to 2.4 ± 0.1 W (total power in two separate output beams) in the visible. The free-running relative intensity noise was measured to be below −55 dBc/Hz over all frequencies from 1 Hz to 1 MHz. With acoustic isolation and temperature regulation of the laser breadboard, the mode-hop free operation time is typically over 5 hrs. To improve the long-term frequency stability, the laser can be locked to a Doppler-free transition of molecular iodine. To estimate the short-term linewidth, the laser was tuned to the resonance of a reference cavity. From analysis of the on-resonance Hänsch-Couillaud error signal we infer a linewidth of 50 ± 10 kHz. Light at 285 nm is generated with an external build-up cavity containing a β-barium borate (BBO) crystal. The UV light is used for loading 25Mg+ ions in a surface-electrode RF Paul trap. These results demonstrate the applicability and versatility of high-power, single-frequency VECSELs with intracavity harmonic generation for applications in atomic and molecular physics.

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Path integral simulation of eigenstates and dynamics of electrons

General information
Thermal desorption of molecular oxygen from SnO$_2$ (110) surface: Insights from first-principles calculations

First-principles density functional theory calculations in the generalized gradient approximation, with plane wave basis set and pseudopotentials, have been used to investigate the desorption pathways of molecular oxygen species adsorbed on the SnO$_2$ (110) surface. Energetics of the thermodynamically favored precursors is studied in dependence on the surface charge provided either by surface defects or by donor type impurities from the near-surface region. The resonant desorption modes of O$_2$ molecules are examined in the framework of ab initio atomic thermodynamics and relationship of these results to experimental observations is discussed.
On the Synthesis, Morphology, and Applications of Engineered Aerosol Nanoparticles

Nanotechnology, the manipulation of matter at the scale of 1–100 nm, is present in everyday life and continues extending into new areas of application. Aerosol synthesis routes, the production of nanoparticles in the gas phase, are known to be continuous, highly controllable, and even suitable for fabricating different types of nanostructured metamaterials—materials with properties not found in nature. In this thesis, single and multicomponent engineered aerosol nanoparticles with different morphologies were synthesized for applications involving interactions between light and matter. The synthesized nanoparticles included spherical silver particles, titania-encapsulated iron oxide particles, silver-decorated silica particles, and silver–titania composite doublet particles. Furthermore, the studied applications for the nanoparticles were magnetically separable photocatalyst nanopowders and nanostructured metal–dielectric metamaterials with linear and nonlinear optical properties, more specifically, localized surface plasmon resonance and second-harmonic generation, respectively.

The aerosol synthesis techniques utilized for the nanoparticle production in this thesis included particle size selection, sintering, encapsulation, and coating. The sintering of the size-selected silver agglomerates to spheres continued the trends found from the literature. In the simple encapsulation process, liquid precursor containing solid particles was sprayed into a tubular furnace where the precursor thermally decomposed on the surface of the solid particles, forming multicomponent particles. This approach was demonstrated by synthesizing titania-encapsulated iron oxide particles. As titania and iron oxide are known to be photocatalytic and magnetic, respectively, the produced nanopowder could find use as a magnetically separable photocatalyst. The silver coatings on the silica and titania carrier particles, accomplished by physical vapor condensation, were found to form different types of morphologies due to the migration of the silver on the carrier particles.

The wavelength of the localized surface plasmon resonance of spherical silver particles deposited on glass substrates was tuned between 400–450 nm with the particle size. Due to the random deposition process, particle–particle contacts on the substrate caused broadening of the extinction spectrum with higher area fractions. On the other hand, the silver-decorated silica nanoparticles maintained the narrow plasmon resonance band even with high particle number densities. This enabled the fabrication of thicker bulk-type optical materials. The nonlinear optical properties of bulk-type multilayer nanostructures consisting of alternating layers of silver-decorated silica nanoparticles and pure silica were investigated. It was proposed that the porous particle layers were in a key role in the formation of the required non-centrosymmetric structure. Furthermore, both the silver particles and the multilayer structure were important for the second-harmonic generation, whose intensity increased with the number of layers. The fabricated structures could be further optimized in order to increase the conversion efficiency of the second-order nonlinear optical process.

Self-subdiffusion in solutions of star-shaped crowders: non-monotonic effects of inter-particle interactions

We examine by extensive computer simulations the self-diffusion of anisotropic star-like particles in crowded two-dimensional solutions. We investigate the implications of the area coverage fraction phi of the crowders and the crowder-
crowder adhesion properties on the regime of transient anomalous diffusion. We systematically compute the mean squared displacement (MSD) of the particles, their time averaged MSD, and the effective diffusion coefficient. The diffusion is ergodic in the limit of long traces, such that the mean time averaged MSD converges towards the ensemble averaged MSD, and features a small residual amplitude spread of the time averaged MSD from individual trajectories. At intermediate time scales, we quantify the anomalous diffusion in the system. Also, we show that the translational-but not rotational-diffusivity of the particles DiS a nonmonotonic function of the attraction strength between them. Both diffusion coefficients decrease as the power law D(\phi) similar to (1 - \phi/\phi*)(2 ... 2.4) with the area fraction \phi occupied by the crowders and the critical value \phi*”. Our results might be applicable to rationalising the experimental observations of non-Brownian diffusion for a number of standard macromolecular crowders used in vitro to mimic the cytoplasmic conditions of living cells.

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Scopus rating (2012): SJR 3.352 SNIP 1.533 CiteScore 3.4
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Scopus rating (2010): SJR 3.395 SNIP 1.421
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Scopus rating (2007): SJR 2.825 SNIP 1.354
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Scopus rating (2005): SJR 1.641 SNIP 1.116
Scopus rating (2004): SJR 1.211 SNIP 1.009
Scopus rating (2003): SJR 1.057 SNIP 0.75
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**Two-step semiclassical model for strong-field ionization with interference and multielectron polarization effects**

We present a semiclassical model for above-threshold ionization with the inclusion of the Stark shift of the initial bound state, the Coulomb potential, and a polarization induced dipole potential capable to describe quantum interference. The model will be used to investigate the imprints of polarization effects in the interference structure of electron momentum distributions.
How large are nonadiabatic effects in atomic and diatomic systems?

With recent developments in simulating nonadiabatic systems to high accuracy, it has become possible to determine how much energy is attributed to nuclear quantum effects beyond zero-point energy. In this work, we calculate the non-relativistic ground-state energies of atomic and molecular systems without the Born-Oppenheimer approximation. For this purpose, we utilize the fixed-node diffusion Monte Carlo method, in which the nodes depend on both the electronic and ionic positions. We report ground-state energies for all systems studied, ionization energies for the first-row atoms and atomization energies for the first-row hydrides. We find the ionization energies of the atoms to be nearly independent of the Born-Oppenheimer approximation, within the accuracy of our results. The atomization energies of molecular systems, however, show small effects of the nonadiabatic coupling between electrons and nuclei.
The critical velocity of rebound determined for sub-micron silver particles with a variable nozzle area impactor

The critical velocity of rebound was determined for spherical silver aerosol particles in the size range of 20-1000 nm. A novel instrument, a variable nozzle area impactor, was especially designed for measuring the particle-surface interaction as a function of the particle impact velocity. The experimental results were combined with a numerical model in order to obtain the impact velocities. The experiments were carried out using a plain aluminum collection substrate in the impactor. Our results show that the critical velocity of rebound decreases from 14 to 0.022 m/s as the particle size increases from 20 to 1000 nm. Furthermore, the critical velocity was found to be proportional to the power of -1.6 of the particle size, instead of the theoretical inverse proportionality. This result is in line with the previous studies for micron-sized particles. In the nanoparticle size range, the obtained values are approximately 3-10 times greater than the recent literature values. This discrepancy can most likely be explained by the different surface materials. All in all, our results give valuable information about the particle-surface interactions in the sub-micron size range.

The critical velocity of rebound determined for sub-micron silver particles with a variable nozzle area impactor

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Quantifying non-ergodic dynamics of force-free granular gases

Brownian motion is ergodic in the Boltzmann-Khinchin sense that long time averages of physical observables such as the mean squared displacement provide the same information as the corresponding ensemble average, even at out-of-equilibrium conditions. This property is the fundamental prerequisite for single particle tracking and its analysis in simple liquids. We study analytically and by event-driven molecular dynamics simulations the dynamics of force-free cooling granular gases and reveal a violation of ergodicity in this Boltzmann-Khinchin sense as well as distinct ageing of the system. Such granular gases comprise materials such as dilute gases of stones, sand, various types of powders, or large molecules, and their mixtures are ubiquitous in Nature and technology, in particular in Space. We treat - depending on the physical-chemical properties of the inter-particle interaction upon their pair collisions - both a constant and a velocity-dependent (viscoelastic) restitution coefficient $\varepsilon$. Moreover we compare the granular gas dynamics with an effective single particle stochastic model based on an underdamped Langevin equation with time dependent diffusivity. We find that both models share the same behaviour of the ensemble mean squared displacement (MSD) and the velocity correlations in the limit of weak dissipation. Qualitatively, the reported non-ergodic behaviour is generic for granular gases with any realistic dependence of $\varepsilon$ on the impact velocity of particles.
Biogenesis of Nascent High Density Lipoprotein Particles

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Scopus rating (2010): SJR 4.628 SNIP 1.468
Scopus rating (2009): SJR 4.761 SNIP 1.462
Scopus rating (2008): SJR 4.212 SNIP 1.377
Scopus rating (2006): SJR 4.11 SNIP 1.485
Real sequence effects on the search dynamics of transcription factors on DNA

Recent experiments show that transcription factors (TFs) indeed use the facilitated diffusion mechanism to locate their target sequences on DNA in living bacteria cells: TFs alternate between sliding motion along DNA and relocation events through the cytoplasm. From simulations and theoretical analysis we study the TF-sliding motion for a large section of the DNA-sequence of a common E. coli strain, based on the two-state TF-model with a fast-sliding search state and a recognition state enabling target detection. For the probability to detect the target before dissociating from DNA the TF-search times self-consistently depend heavily on whether or not an auxiliary operator (an accessible sequence similar to the main operator) is present in the genome section. Importantly, within our model the extent to which the interconversion rates between search and recognition states depend on the underlying nucleotide sequence is varied. A moderate dependence maximises the capability to distinguish between the main operator and similar sequences. Moreover, these auxiliary operators serve as starting points for DNA looping with the main operator, yielding a spectrum of target detection times spanning several orders of magnitude. Auxiliary operators are shown to act as funnels facilitating target detection by TFs.

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Authors: Bauer, M., Rasmussen, E. S., Lomholt, M. A., Metzler, R.
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Phase State and Deliquescence Hysteresis of Ammonium-Sulfate-Seeded Secondary Organic Aerosol

The phase state of secondary organic aerosol (SOA) has an impact on its lifetime, composition, and its interaction with water. To better understand the effect of phase state of SOA on climate interactions, we studied the SOA phase state and the effect of its history and report here the phase state and the humidity-induced phase hysteresis of multicomponent-seeded SOA particles produced in a large, continuously stirred tank reactor. We determined the phase state of the particles by their bounced fraction impacting on a smooth substrate in a low-pressure impactor. The particles were composed of ammonium sulfate ([NH4](2)SO4) seed and a secondary organic matter (SOM) shell formed from oxidized alpha-pinene or isoprene. The ammonium sulfate (AS) seed dominated the deliquescence of the alpha-pinene SOM multicomponent particles, whereas their efflorescence was strongly attenuated by the SOM coating. Particles coated with isoprene SOM showed continuous phase transitions with a lesser effect by the AS seed. The results agree with and independently corroborate contemporary research.

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Studies of Physical Phase State of Aerosol Nanoparticles

Aerosol particles produced in the atmosphere have major effects on the life on Earth: cloud formation starts on seed particles, often formed by photochemical oxidation of biogenic volatile organic compounds; visibility, corrosion, and health problems are caused by anthropogenic hydrocarbon and sulfur emission processed into particles by the atmosphere and the sun.

Naturally occurring secondary organic aerosol (SOA) particles can produce up to a half of the non-refractory mass of aerosol particles of less than micrometer in size. This makes SOA a large contributing factor to the climate system of the Earth. The actual effect that these particles have is, however, not well known, compared to the other effects affecting the climate. The research effort to increase the understanding and reduce the uncertainties around the climate effects of SOA encompasses an interdisciplinary research community.

The recent advance made by the observation of a solid phase of SOA by Virtanen et al. (2010) was the starting point for this thesis. The solid phase of SOA particles means that a long-held assumption of a partition equilibrium between the condensed phase and the gas phase of the semivolatile species may be wrong and produce too low a timescale for the particle chemical reaction rates and uptake coefficients.

This work consists of new developments in the instrumentation of particle properties as well as new observations of laboratory-generated secondary organic aerosol. The method development has two branches, one concentrates on finding more information from the measurement signal of an electrical low pressure impactor (ELPI) used in a somewhat unconventional way, whereas the other consists of a new detection method for particle bounce and response to different humidity and phase hysteresis induced by a carefully controlled humidity history.

The methods and observations made during this work are by no means the final word on the subject, but they are being used and further developed by the scientific community. Study of the particle phase and bounce as well as SOA mechanical properties and kinetics is well underway, and its results will be used to further refine the understanding of both aerosol fundamentals as well as the climate system.
vibrational contributions can be evaluated either separately or simultaneously. Indeed, at finite temperature and non-zero-field strengths we observe considerable rovibrational effects in the polarization of the hydrogen molecule. Given sufficient computational resources, the path-integral Monte Carlo method turns out to be a straightforward tool for describing and computing static polarizabilities for traditionally challenging regimes.

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Source-ID: urn:069084BC266EF8BB0195BF85DD7DD69
Research output: Scientific - peer-review » Article

Workplace performance of a loose-fitting powered air purifying respirator during nanoparticle synthesis
Nanoparticle (particles with diameter ≤100 nm) exposure is recognized as a potentially harmful size fraction for pulmonary particle exposure. During nanoparticle synthesis, the number concentrations in the process room may exceed 10 × 10<sup>6</sup> cm<sup>-3</sup>. During such conditions, it is essential that the occupants in the room wear highly reliable high-performance respirators to prevent inhalation exposure. Here we have studied the in-use program protection factor (PPF) of loose-fitting powered air purifying respirators, while workers were coating components with TiO<inf>2</inf> or Cu<inf>x</inf>O<inf>y</inf> nanoparticles under a hood using a liquid flame spray process. The PPF was measured using condensation particle counters, an electrical low pressure impactor, and diffusion chargers. The room particle concentrations varied from 4 × 10<sup>4</sup> to 40 × 10<sup>6</sup> cm<sup>-3</sup>, and the count median aerodynamic diameter ranged from 32 to 180 nm. Concentrations inside the respirator varied from 0.7 to 7.2 cm<sup>-3</sup>. However, on average, tidal breathing was assumed to increase the respirator concentration by 2.3 cm<sup>-3</sup>. The derived PPF exceeded 1.1 × 10<sup>4</sup>, which is more than 40 × 10<sup>3</sup>
times the respirator assigned protection factor. We were unable to measure clear differences in the PPF of respirators with old and new filters, among two male and one female user, or assess most penetrating particle size. This study shows that the loose-fitting powered air purifying respirator provides very efficient protection against nanoparticle inhalation exposure if used properly.

**General information**

**State:** Published
**Ministry of Education publication type:** A1 Journal article-refereed
**Organisations:** Department of Physics, Research group: Aerosol Synthesis, National Research Centre for the Working Environment, Finnish Institute of Occupational Health, Helsinki University, TNO
**Authors:** Koivisto, A. J., Aromaa, M., Koponen, I. K., Fransman, W., Jensen, K. A., Mäkelä, J. M., Hämeri, K. J.
**Publication date:** 9 Apr 2015
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- Scopus rating (2014): SJR 0.663 SNIP 0.868 CiteScore 2.17
- Scopus rating (2013): SJR 0.749 SNIP 1.013 CiteScore 2.54
- Scopus rating (2012): SJR 0.855 SNIP 1.03 CiteScore 2.56
- Scopus rating (2011): SJR 1.09 SNIP 1.44 CiteScore 3.52
- Scopus rating (2010): SJR 0.966 SNIP 1.248
- Scopus rating (2009): SJR 0.977 SNIP 1.053
- Scopus rating (2008): SJR 0.989 SNIP 1.138
- Scopus rating (2007): SJR 0.873 SNIP 1.082
- Scopus rating (2006): SJR 0.862 SNIP 1.242
- Scopus rating (2005): SJR 0.805 SNIP 1.174
- Scopus rating (2004): SJR 0.805 SNIP 1.332
- Scopus rating (2003): SJR 0.564 SNIP 0.87
- Scopus rating (2002): SJR 0.676 SNIP 1.226
- Scopus rating (2001): SJR 0.503 SNIP 0.653
- Scopus rating (2000): SJR 0.296 SNIP 0.409
**Original language:** English
**ASJC Scopus subject areas:** Atomic and Molecular Physics, and Optics, Condensed Matter Physics, Modelling and Simulation, Chemistry(all), Materials Science(all), Bioengineering
**Keywords:** Aerosol, Air purifying respirator, Filtration, Occupational safety, Protection factor, Respirator performance

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- http://www.scopus.com/inward/record.url?scp=84927730047&partnerID=8YFLogxK (Link to publication in Scopus)

**Bibliographical note**

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**Source:** Scopus
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**Research output:** Scientific - peer-review » Article

**Conformational properties of complex polymers: Rosette versus star-like structures**

Multiple loop formation in polymer macromolecules is an important feature of the chromatin organization and DNA compaction in the nuclei. We analyse the size and shape characteristics of complex polymer structures, containing in general $f_{\text{inf}}^1<1</inf>$ loops (petals) and $f_{\text{inf}}^2<2</inf>$ linear chains (branches). Within the frames of continuous model of Gaussian macromolecule, we apply the path integration method and obtain the estimates for gyration radius $R<\text{inf}>g</inf>$ and asphericity $A$ of typical conformation as functions of parameters $f_{\text{inf}}^1<1</inf>$, $f_{\text{inf}}^2<2</inf>$. In particular, our results qualitatively reveal the extent of anisotropy of star-like topologies as compared to the rosette structures of the same total molecular weight.
Polymer looping is controlled by macromolecular crowding, spatial confinement, and chain stiffness

We study by extensive computer simulations the looping characteristics of linear polymers with varying persistence length inside a spherical cavity in the presence of macromolecular crowding. For stiff chains, the looping probability and looping time reveal wildly oscillating patterns as functions of the chain length. The effects of crowding differ dramatically for flexible versus stiff polymers. While for flexible chains the looping kinetics is slowed down by the crowders, for stiffer chains the kinetics turns out to be either decreased or facilitated, depending on the polymer length. For severe confinement, the looping kinetics may become strongly facilitated by crowding. Our findings are of broad impact for DNA looping in the crowded and compartmentalized interior of living biological cells.
Proton-coupled electron transfer and the role of water molecules in proton pumping by cytochrome c oxidase

Molecular oxygen acts as the terminal electron sink in the respiratory chains of aerobic organisms. Cytochrome c oxidase in the inner membrane of mitochondria and the plasma membrane of bacteria catalyzes the reduction of oxygen to water, and couples the free energy of the reaction to proton pumping across the membrane. The proton-pumping activity contributes to the proton electrochemical gradient, which drives the synthesis of ATP. Based on kinetic experiments on the O-O bond splitting transition of the catalytic cycle (A → PR), it has been proposed that the electron transfer to the binuclear iron-copper center of O2 reduction initiates the proton pump mechanism. This key electron transfer event is coupled to an internal proton transfer from a conserved glutamic acid to the proton-loading site of the pump. However, the proton may instead be transferred to the binuclear center to complete the oxygen reduction chemistry, which would constitute a short-circuit. Based on atomistic molecular dynamics simulations of cytochrome c oxidase in an explicit membrane-solvent environment, complemented by related free-energy calculations, we propose that this short-circuit is effectively prevented by a redoxstate-dependent organization of water molecules within the protein structure that gates the proton transfer pathway. cell respiration , atomistic molecular dynamics simulations , functional water molecules ,free-energy calculations .
Real-space Wigner-Seitz Cells Imaging of Potassium on Graphite via Elastic Atomic Manipulation

Atomic manipulation in the scanning tunnelling microscopy, conventionally a tool to build nanostructures one atom at a time, is here employed to enable the atomic-scale imaging of a model low-dimensional system. Specifically, we use low-temperature STM to investigate an ultra thin film (4 atomic layers) of potassium created by epitaxial growth on a graphite substrate. The STM images display an unexpected honeycomb feature, which corresponds to a real-space visualization of the Wigner-Seitz cells of the close-packed surface K atoms. Density functional simulations indicate that this behaviour arises from the elastic, tip-induced vertical manipulation of potassium atoms during imaging, i.e. elastic atomic manipulation, and reflects the ultrasoft properties of the surface under strain. The method may be generally applicable to other soft e.g. molecular or biomolecular systems.
Silver sulfide nanoclusters and the superatom model

The superatom model of electron-shell closings has been widely used to explain the stability of noble-metal nanoclusters of few nanometers, including thiolate-protected Au and Ag nanoclusters. The presence of core sulfur atoms in silver sulfide (Ag-S) nanoclusters renders them a class of clusters with distinctive properties as compared to typical noble-metal clusters. Here, it is natural to ask whether the superatom model is still applicable for the Ag-S nanoclusters with mixed metal and nonmetal core atoms. To address this question, we applied density functional simulations to analyze a series of Ag-S nanoclusters: Ag_{14}S(SPh)_{12}(PPh_{3})_{8}, Ag_{14}(SC_{6}H_{5}F_{2})_{12}(PPh_{3})_{8}, Ag_{70}S_{16}(SPh)_{34}(PhCO_{2})_{4}(triphos)_{4}, and [Ag_{123}S_{35}(StBu)_{50}]^{3+}. We observed that superatomic orbitals are still present in the conduction band of these Ag-S clusters where the cluster cores comprise mostly silver atoms. Our Bader charge analysis illustrates that thiolates play a significant role in withdrawing charge (electron density) from the core Ag atoms. The simulated optical absorption properties of the selected Ag-S clusters reflect the substantial band gaps associated with typical molecular orbitals on both sides. Apart from Ag_{14}S(SPh)_{12}(PPh_{3})_{8}, which has a central sulfur atom in the cluster core, superatomic orbitals of the Ag-S clusters can have contributions for individual transitions in the conduction band.

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Organisations: Department of Physics, Research group: Materials and Molecular Modeling, Computational Science X (CompX), University of Jyväskylä, Departments of Physics and Chemistry
Authors: Goh, J., Malola, S., Häkkinen, H., Akola, J.
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Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
Scopus rating (2010): SJR 2.438 SNIP 1.356
Scopus rating (2009): SJR 2.128 SNIP 1.417
Scopus rating (2008): SJR 1.856 SNIP 1.033
Original language: English
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Electronic, Optical and Magnetic Materials, Surfaces, Coatings and Films, Energy(all)
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Research output: Scientific - peer-review › Article

Weak ergodicity breaking and ageing in anomalous diffusion

General information
Detection of the relativistic electrons at atmosphere

General information
State: Published
Ministry of Education publication type: D3 Professional conference proceedings
Organisations: Department of Physics, Sodankylä Geophysical Observatory FIN-99600 Sodankylä Finland
Authors: Gholizadehkalkhoran, H., Turunen, E.
Publication date: 2015

Host publication information
Title of host publication: FINCOSPAR 2015
Links:
http://www.cospar.fi/fincospar2015/
Research output: Professional › Conference contribution

Fluorescence-based Real-Time Characterization of Bioaerosols

General information
State: Published
Ministry of Education publication type: G5 Doctoral dissertation (article)
Organisations: Department of Physics, Research area: Aerosol Physics
Authors: Saari, S.
Number of pages: 53
Publication date: 2015

Publication information
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Publisher: Tampere University of Technology
Geometry controlled anomalous diffusion in random fractal geometries: Looking beyond the infinite cluster

We investigate the ergodic properties of a random walker performing (anomalous) diffusion on a random fractal geometry. Extensive Monte Carlo simulations of the motion of tracer particles on an ensemble of realisations of percolation clusters are performed for a wide range of percolation densities. Single trajectories of the tracer motion are analysed to quantify the time averaged mean squared displacement (MSD) and to compare this with the ensemble averaged MSD of the particle motion. Other complementary physical observables associated with ergodicity are studied, as well. It turns out that the time averaged MSD of individual realisations exhibits non-vanishing fluctuations even in the limit of very long observation times as the percolation density approaches the critical value. This apparent non-ergodic behaviour concurs with the ergodic behaviour on the ensemble averaged level. We demonstrate how the non-vanishing fluctuations in single particle trajectories are analytically expressed in terms of the fractal dimension and the cluster size distribution of the random geometry, thus being of purely geometrical origin. Moreover, we reveal that the convergence scaling law to ergodicity, which is known to be inversely proportional to the observation time T for ergodic diffusion processes, follows a power-law $\sim T^{-h}$ with $h < 1$ due to the fractal structure of the accessible space. These results provide useful measures for differentiating the subdiffusion on random fractals from an otherwise closely related process, namely, fractional Brownian motion. Implications of our results on the analysis of single particle tracking experiments are provided.
Light-Induced Waveguides in Nematic Liquid Crystals

Spatial optical solitary waves in media with nonlinear refractive index are self-localized beams as well as waveguides induced by light. We review their guiding features in reorientational birefringent soft matter, namely nematic liquid crystals, for which a highly "nonlocal" response enhances the confinement, stabilization, and robustness of the generated optical solitary waves, termed "nematicons." The waveguiding properties of the spatial solitons in nematic liquid crystals are illustrated through the confinement of low-power signals and other solitary waves, as well as optical vortices.

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Authors: Assanto, G., Smyth, N. F.
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Scopus rating (2015): SJR 1.449 SNIP 1.393 CiteScore 3.03
Scopus rating (2014): SJR 1.889 SNIP 2.072 CiteScore 3.49
Scopus rating (2013): SJR 2.258 SNIP 2.38 CiteScore 4.55
Scopus rating (2012): SJR 2.742 SNIP 2.661 CiteScore 4.35
Scopus rating (2011): SJR 2.367 SNIP 2.845 CiteScore 3.87
Scopus rating (2010): SJR 2.217 SNIP 2.599
Scopus rating (2009): SJR 2.964 SNIP 2.869
Scopus rating (2008): SJR 2.476 SNIP 2.433
Scopus rating (2007): SJR 2.428 SNIP 1.746
Scopus rating (2006): SJR 2.131 SNIP 2.383
Scopus rating (2005): SJR 2.93 SNIP 2.594
Scopus rating (2004): SJR 2.827 SNIP 2.62
Scopus rating (2003): SJR 3.121 SNIP 3.103
Scopus rating (2002): SJR 2.664 SNIP 2.508
Scopus rating (2001): SJR 2.25 SNIP 1.926
Scopus rating (2000): SJR 2.37 SNIP 1.335
Scopus rating (1999): SJR 3.466 SNIP 1.611
Original language: English
ASJC Scopus subject areas: Electrical and Electronic Engineering, Atomic and Molecular Physics, and Optics
Keywords: Liquid crystals, Nonlinear optics, Optical solitons, Optical vortices, Solitons
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http://www.scopus.com/inward/record.url?scp=84941047633&partnerID=8YFLogxK (Link to publication in Scopus)
Source: Scopus
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Memory effect in crystallization of amorphous Ge2Sb2Te5

The Prototype Phase Change Material Ge2Sb2Te5: Amorphous structure and crystallization

The widespread use of phase change materials in storage media is based on the extremely rapid and reversible switching between the amorphous and crystalline phases of some families of semiconducting alloys. Detailed information about the structure of the amorphous phase and the mechanism of crystallization are essential for the development of new storage media, and we study both aspects here using density functional/molecular dynamics simulations of Ge\(^2\)Sb\(^2\)Te\(^5\), the prototype phase change material of the Ge/Sb/Te semiconductor family.

Van der Waals interactions are critical in Car-Parrinello molecular dynamics simulations of porphyrin-fullerene dyads

The interplay between electrostatic and van der Waals (vdW) interactions in porphyrin-C\(_{60}\) dyads is still under debate despite its importance in influencing the structural characteristics of such complexes considered for various applications in molecular photovoltaics. In this article, we sample the conformational space of a porphyrin-C\(_{60}\) dyad using Car-Parrinello molecular dynamics simulations with and without empirical vdW corrections. Long-range vdW interactions, which are poorly described by the commonly used density functional theory functionals, prove to be essential for a proper dynamics of the dyad moieties. Inclusion of vdW corrections brings porphyrin and C\(_{60}\) close together in an orientation that is in agreement with experimental observations. The structural differences arising from the vdW corrections are shown to be significant for several properties and potentially less important for others. Additionally, our Mulliken population analysis reveals that contrary to the common belief, porphyrin is not the primary electron donating moiety for C\(_{60}\). In the considered dyad, fullerene's affinity for electrons is primarily satisfied by charge transfer from the amide group of the
linker. However, we show that in the absence of another suitable bound donor, C\textsubscript{60} can withdraw electrons from porphyrin if it is sufficiently close.

**General information**

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**Organisations:** Department of Physics, Research area: Computational Physics, Department of Chemistry and Bioengineering, Research group: Supramolecular photochemistry, Computational Science X (CompX), Frontier Photonics, VTT Technical Research Centre of Finland  
**Authors:** Karilainen, T., Cramariuc, O., Kuisma, M., Tappura, K., Hukka, T. I.  
**Number of pages:** 10  
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**Publication information**

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**Ratings:**  
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Scopus rating (2015): SJR 1.417 SNIP 1.451 CiteScore 3.81  
Scopus rating (2014): SJR 1.489 SNIP 1.451 CiteScore 3.78  
Scopus rating (2013): SJR 1.449 SNIP 1.516 CiteScore 4.15  
Scopus rating (2012): SJR 1.874 SNIP 1.64 CiteScore 4.43  
Scopus rating (2011): SJR 1.834 SNIP 1.611 CiteScore 4.47  
Scopus rating (2010): SJR 1.745 SNIP 1.366  
Scopus rating (2009): SJR 1.859 SNIP 1.208  
Scopus rating (2008): SJR 2.482 SNIP 1.655  
Scopus rating (2007): SJR 2.789 SNIP 1.794  
Scopus rating (2006): SJR 2.201 SNIP 1.561  
Scopus rating (2005): SJR 1.912 SNIP 1.373  
Scopus rating (2004): SJR 1.695 SNIP 1.321  
Scopus rating (2003): SJR 1.666 SNIP 1.402  
Scopus rating (2002): SJR 1.524 SNIP 1.138  
Scopus rating (2001): SJR 1.711 SNIP 1.237  
Scopus rating (2000): SJR 1.693 SNIP 1.215  
Scopus rating (1999): SJR 1.626 SNIP 1.423  
**Original language:** English  
**Keywords:** Car-Parrinello molecular dynamics, Fullerene, Porphyrin, Time-dependent-density functional theory  
**ASJC Scopus subject areas:** Chemistry(all), Computational Mathematics  
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http://www.scopus.com/inward/record.url?scp=84923259668&partnerID=8YFLogxK (Link to publication in Scopus)

**Bibliographical note**

ORG=fys,0.5  
ORG=keb,0.5  
Source: Scopus  
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Research output: Scientific - peer-review › Article

**Vedyn Stark-ilmiön ja polarisoituvuksien mallintaminen polkuintegraali-Monte Carlo-menetelmällä**

Ulkoisen sähkökentän vaikutusta kvanttimekaaniseen kuvaukseen mallinnetaan käyttämällä polarisoituvuutta, jonka eri komponentit kuvaavat myös aineen optisia ominaisuuksia. Näistä staattinen dipolipolarisoituvuus α sekä hyperpolarisoituvuudet β, γ... liittyvät keskeisesti Stark-ilmiön eli ominaislojen energiaspektreen silpoutumiseen sähkökentässä. Tässä tutkimuksessa tarkastellaan äärellisen sähkökentän simuloinmiseen ja staattisten polarisoituvuuksien laskemiseen liittyvää problematikkaa, jota lähestytään ensimmäistä kertaa suorana äärellisessä lämpötilassa käyttämällä polkuintegraali-Monte Carlo -menetelmää (PIMC). Sähkökentän kuvaaminen käsitellään yksityiskohtaisesti ja sitä sovelletaan Finite field-periaatteella neljään eri vetyyksysteemiin: H, H\textsuperscript{+}, H\textsubscript{2}\textsuperscript{+} ja H\textsubscript{2}. Menetelmä
toimii luotettavasti, ja saadut tulokset vastaavat tunnettujia staattisten polarisoituvuuksien arvoja erinomaisesti sekä
adiabaattisissa että ei-adiabaattisissa tapauksissa. Lisäksi merkittävä äärellinen lämpötilan vaikutus havaitaan
vetymolekyyleillä, joilla rotaatio- ja vibraatiotilojen osuudet ovat suuret. Laskentakapasiteetin riittäessä PIMC-menetelmä
voidaan todeta suoraviivaisena keinoiksi staattisten polarisoituvuuksien kuvaamiseen ja laskemiseen äärellisissä
lämpötiloissa myös niissä tapauksissa, joissa perinteiset menetelmät osoittautuvat työläiksi.

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Authors: Tiihonen, J.
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Publication date: 3 Sep 2014

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Original language: Finnish
Keywords: path integral Monte Carlo, finite temperature, quantum statistics, polarizability, hyperpolarizability, hydrogen
ASJC Scopus subject areas: Atomic and Molecular Physics, and Optics
Electronic versions:
Juha Tiihonen - Diplomityö
Links:
http://urn.fi/URN:NBN:fi:tty-201410301532
Research output: Scientific › Master's Thesis

Asymmetric photoelectron momentum distributions due to quantum interference in strong-field ionization by a few-cycle pulse

General information
State: Published
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Organisations: Research area: Computational Physics, Research group: Quantum Control and Dynamics, Department of
Physics, Computational Science X (CompX)
Authors: Shvetsov-Shilovski, N. I., Räsänen, E., Paulus, G. G., Madsen, L. B.
Number of pages: 10
Pages: 043431-1 - 043431-10
Publication date: 2014
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Scopus rating (2013): SJR 2.317 SNIP 1.179 CiteScore 2.86
Scopus rating (2012): SJR 2.515 SNIP 1.239 CiteScore 2.81
Scopus rating (2011): SJR 2.31 SNIP 1.261 CiteScore 2.79
Scopus rating (2010): SJR 2.403 SNIP 1.22
Scopus rating (2009): SJR 2.475 SNIP 1.305
Scopus rating (2008): SJR 2.559 SNIP 1.241
Scopus rating (2007): SJR 2.618 SNIP 1.259
Scopus rating (2006): SJR 2.342 SNIP 1.257
Scopus rating (2005): SJR 2.017 SNIP 1.286
Scopus rating (2004): SJR 2.168 SNIP 1.1
Scopus rating (2003): SJR 2.05 SNIP 1.078
Scopus rating (2002): SJR 2.037 SNIP 1.191
Chalcopyrite quantum wells and dots in solar-cell applications

Chalcopyrite structures are promising candidates for efficient advanced solar cells in thin-film technology. Here we discuss the nanostructuring approach to thin-film photovoltaics and introduce the benefits and challenges of chalcopyrite materials for that purpose. We focus on chalcopyrite quantum wells and quantum dots by describing in detail the growth procedure as well as the theoretical modeling of the obtained structures. We demonstrate that both quantum wells and dots have, in principle, desirable characteristics for applications in photovoltaics.

Hybrid systems of AlInP microdisks and colloidal CdSe nanocrystals showing whispering-gallery modes at room temperature

We report on the realization of hybrid systems composed of passive optical microdisk resonators prepared from epitaxial layer systems and nanocrystal quantum emitters synthesized by colloidal chemistry. The AlInP disk material allows for the operation in the visible range, as probed by CdSe-based nanocrystals. Photoluminescence spectra at room temperature reveal sets of whispering-gallery modes consistent with finite-difference time-domain simulations. In the experiments, a special sample geometry renders it possible to detect resonant optical modes perpendicular to the disk plane.
Optimal control of high-harmonic generation by intense few-cycle pulses

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Quantum Control and Dynamics, Department of Physics, Computational Science X (CompX)
Authors: Solanpää, J., Budagosky, J., Shvetsov-Shilovski, N., Castro, A., Rubio, A., Räsänen, E.
Number of pages: 5
Pages: 1-5
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Scopus rating (2015): SJR 1.451 SNIP 0.903 CiteScore 2.06
Scopus rating (2014): SJR 2.121 SNIP 1.146 CiteScore 2.46
Scopus rating (2013): SJR 2.317 SNIP 1.179 CiteScore 2.86
Scopus rating (2012): SJR 2.515 SNIP 1.239 CiteScore 2.81
Scopus rating (2011): SJR 2.31 SNIP 1.261 CiteScore 2.79
Scaling in the correlation energies of atomic ions

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Quantum Control and Dynamics, Department of Physics, Computational Science X (CompX)
Authors: Odriazola, A., Gonzalez, A., Räsänen, E.
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Scopus rating (2014): SJR 2.121 SNIP 1.146 CiteScore 2.46
Scopus rating (2013): SJR 2.317 SNIP 1.179 CiteScore 2.86
Scopus rating (2012): SJR 2.515 SNIP 1.239 CiteScore 2.81
Scopus rating (2011): SJR 2.31 SNIP 1.261 CiteScore 2.79
Scopus rating (2010): SJR 2.403 SNIP 1.22
Scopus rating (2009): SJR 2.475 SNIP 1.305
Scopus rating (2008): SJR 2.559 SNIP 1.241
Scopus rating (2007): SJR 2.618 SNIP 1.259
Scopus rating (2006): SJR 2.342 SNIP 1.257
Scopus rating (2005): SJR 2.017 SNIP 1.286
Scopus rating (2004): SJR 2.168 SNIP 1.1
Scopus rating (2003): SJR 2.05 SNIP 1.078
Stable and efficient momentum-space solutions of the time-dependent Schrödinger equation for one-dimensional atoms in strong laser fields

General information
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Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Quantum Control and Dynamics, Department of Physics, Computational Science X (CompX)
Authors: Shvetsov-Shilovski, N. I., Räsänen, E.
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Pages: 174-181
Publication date: 2014
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Volume: 279
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Scopus rating (2015): SJR 2.098 SNIP 1.988 CiteScore 2.92
Scopus rating (2014): SJR 2.166 SNIP 2.193 CiteScore 3.12
Scopus rating (2013): SJR 2.227 SNIP 2.45 CiteScore 3.3
Scopus rating (2012): SJR 2.161 SNIP 2.052 CiteScore 2.69
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