Investigation of the structural anisotropy in a self-assembling glycinate layer on Cu(100) by scanning tunneling microscopy and density functional theory calculations

Self-assembling organic molecule-metal interfaces exhibiting free-electron like (FEL) states offers an attractive bottom-up approach to fabricating materials for molecular electronics. Accomplishing this, however, requires detailed understanding of the fundamental driving mechanisms behind the self-assembly process. For instance, it is still unresolved as to why the adsorption of glycine ([NH2(CH2)COOH]) on isotropic Cu(100) single crystal surface leads, via deprotonation and self-assembly, to a glycinate ([NH2(CH2)COO−]) layer that exhibits anisotropic FEL behavior. Here, we report on bias-dependent scanning tunneling microscopy (STM) experiments and density functional theory (DFT) calculations for glycine adsorption on Cu(100) single crystal surface. We find that after physical vapor deposition (PVD) of glycine on Cu(100), glycinate self-assembles into an overlayer exhibiting c(2x4) and p(2x4) symmetries with non-identical adsorption sites. Our findings underscore the intricacy of electrical conductivity in nanomolecular organic overlayers and the critical role the structural anisotropy at molecule-metal interface plays in the fabrication of materials for molecular electronics.

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Authors: Kuzmin, M., Lahtonen, K., Vuori, L., Sánchez-de-Armas, R., Hirsimäki, M., Valden, M.
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Scopus rating (2015): 0.914 1.3
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Publication Forum (2015): 1
Scopus rating (2014): 0.958 1.477
Web of Science (2014): 2.711 2.735 5.3 0.507 0.07467 0.549
Publication Forum (2014): 2
Scopus rating (2013): 0.965 1.488
Publication Forum (2013): 2
Scopus rating (2012): 0.918 1.373
Publication Forum (2012): 2
Scopus rating (2011): 0.908 1.402
Scopus rating (2010): 0.924 1.141
Scopus rating (2009): 0.842 1.023
Scopus rating (2008): 0.899 1.087
Scopus rating (2007): 0.795 0.945
Scopus rating (2006): 0.852 1.052
Scopus rating (2005): 0.679 0.946
Scopus rating (2004): 0.964 1.126
Scopus rating (2003): 0.988 1.027
Scopus rating (2002): 0.921 0.954
Scopus rating (2001): 0.841 0.796
Scopus rating (2000): 0.866 0.772
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Lipid membranes: Theory and simulations bridged to experiments

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Organisations: Department of Physics, University of Helsinki, MEMPHYS - Centre for Biomembrane Physics, University of Southern Denmark
Authors: Vattulainen, I., Róg, T.
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ASJC Scopus subject areas: Biophysics, Biochemistry, Cell Biology

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Web of Science (2015): 3.687 3.589 7.3 0.907 0.02731 1.163
Publication Forum (2015): 1
Scopus rating (2014): 1.869 1.09
Web of Science (2014): 3.836 3.881 7.0 1.006 0.02991 1.257
Publication Forum (2014): 2
Scopus rating (2013): 1.592 0.975
Publication Forum (2013): 2
Scopus rating (2012): 1.833 1.156
Publication Forum (2012): 2
Scopus rating (2011): 1.644 1.227
Scopus rating (2009): 2.152 1.298
Scopus rating (2008): 2.035 1.123
Scopus rating (2007): 2.021 1.158
Scopus rating (2005): 2.037 1.231
Scopus rating (2004): 1.5 1.147
Scopus rating (2003): 1.401 1.115
Scopus rating (2002): 1.594 1.228
Scopus rating (2001): 1.509 1.053
Scopus rating (2000): 1.089 0.907
Scopus rating (1999): 0.95 0.841
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Research output: Scientific - peer-review › Editorial
Cholesterol oxidation products and their biological importance

The main biological cause of oxysterols is the oxidation of cholesterol. They differ from cholesterol by the presence of additional polar groups that are typically hydroxyl, keto, hydroperoxy, epoxy, or carboxyl moieties. Under typical conditions, oxysterol concentration is maintained at a very low and precisely regulated level, with an excess of cholesterol. Like cholesterol, many oxysterols are hydrophobic and hence confined to cell membranes. However, small chemical differences between the sterols can significantly affect how they interact with other membrane components, and this in turn can have a substantial effect on membrane properties. In this spirit, this review describes the biological importance and the roles of oxysterols in the human body. We focus primarily on the effect of oxysterols on lipid membranes, but we also consider other issues such as enzymatic and nonenzymatic synthesis processes of oxysterols as well as pathological conditions induced by oxysterols.

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Organisations: Department of Physics, Research area: Computational Physics, Research group: Biological Physics and Soft Matter, J. Heyrovsky Institute of Physical Chemistry, Academy of Sciences of the Czech Republic
Authors: Kulig, W., Cwiklik, L., Jurkiewicz, P., Rog, T., Vattulainen, I.
Keywords: (Biological membranes, Biophysical properties, Cholesterol, Oxidation, Oxidative stress, Oxysterols, Reactive oxygen species)
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ASJC Scopus subject areas: Biochemistry, Molecular Biology, Organic Chemistry, Cell Biology

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Scopus rating (2016): 0.976 0.862
Publication Forum (2016): 1
Scopus rating (2015): 0.957 0.957
Web of Science (2015): 2.901 2.75 >10.0 0.868 0.00491 0.736
Publication Forum (2015): 1
Scopus rating (2014): 0.885 1.039
Web of Science (2014): 2.422 2.697 >10.0 1.233 0.00529 0.788
Publication Forum (2014): 1
Scopus rating (2013): 0.82 1.055
Publication Forum (2013): 1
Scopus rating (2012): 0.803 0.974
Publication Forum (2012): 1
Scopus rating (2011): 0.727 0.984
Scopus rating (2010): 0.874 0.964
Scopus rating (2009): 0.9 0.995
Scopus rating (2008): 1.114 1.057
Scopus rating (2007): 1.083 1.091
Scopus rating (2006): 0.808 0.881
Scopus rating (2005): 1.038 1.035
Scopus rating (2004): 0.69 0.831
Scopus rating (2003): 0.917 0.817
Scopus rating (2002): 1.005 0.813
Scopus rating (2001): 1.097 0.827
Scopus rating (2000): 0.738 0.742
Scopus rating (1999): 0.737 0.705
Original language: English
DOIs:
Exercise loading history and femoral neck strength in a sideways fall: A three-dimensional finite element modeling study.

Over 90% of hip fractures are caused by falls. Due to a fall-induced impact on the greater trochanter, the posterior part of the thin superolateral cortex of the femoral neck is known to experience the highest stress, making it a fracture-prone region. Cortical geometry of the proximal femur, in turn, reflects a mechanically appropriate form with respect to habitual exercise loading. In this finite element (FE) modeling study, we investigated whether specific exercise loading history is associated with femoral neck structural strength and estimated fall-induced stresses along the femoral neck. One hundred and eleven three-dimensional (3D) proximal femur FE models for a sideways falling situation were constructed from magnetic resonance (MR) images of 91 female athletes (aged 24.7±6.1years, >8years competitive career) and 20 non-competitive habitually active women (aged 23.7±3.8years) that served as a control group. The athletes were divided into five distinct groups based on the typical loading pattern of their sports: high-impact (H-I: triple-jumpers and high-jumpers), odd-impact (O-I: soccer and squash players), high-magnitude (H-M: power-lifters), repetitive-impact (R-I: endurance runners), and repetitive non-impact (R-NI: swimmers). The von Mises stresses obtained from the FE models were used to estimate mean fall-induced stresses in eight anatomical octants of the cortical bone cross-sections at the proximal, middle, and distal sites along the femoral neck axis. Significantly (p<0.05) lower stresses compared to the control group were observed: the H-I group - in the superoposterior (10%) and posterior (19%) octants at the middle site, and in the superoposterior (13%) and posterior (22%) octants at the distal site; the O-I group - in the superoposterior (16%), superoposterior (16%), and posterior (12%) octants at the middle site, and in the superoposterior (14%) octant at the distal site; the H-M group - in the superior (13%) and superoposterior (15%) octants at the middle site, and a trend (p=0.07, 9%) in the superoposterior octant at the distal site; the R-I group - in the superior (14%), superoposterior (23%) and posterior (22%) octants at the middle site, and in the superoposterior (19%) and posterior (20%) octants at the distal site. The R-NI group did not differ significantly from the control group. These results suggest that exercise loading history comprising various impacts in particular is associated with a stronger femoral neck in a falling situation and may have potential to reduce hip fragility.

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Organisations: Department of Mechanical Engineering and Industrial Systems, Research area: Applied Mechanics, Department of Electronics and Communications Engineering, Research group: Computational Biophysics and Imaging Group, BioMediTech, UK Inst Hlth Promot Res, UK Institute, University of Jyväskylä
Authors: Abe, S., Narra, N., Nikander, R., Hyttinen, J., Kouhia, R., Sievänen, H.
Keywords: (Bone strength, Finite element analysis, Exercise , Falling , OSTEOPOROSIS, Hip fracture)
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ASJC Scopus subject areas: Orthopedics and Sports Medicine, Biochemistry, medical, Physical Therapy, Sports Therapy and Rehabilitation

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Web of Science (2015): 3.736 4.146 7.9 0.764 0.0347 1.36
Publication Forum (2015): 2
Scopus rating (2014): 1.794 1.656
Web of Science (2014): 3.973 4.312 7.5 0.774 0.0356 1.333
Publication Forum (2014): 2
Scopus rating (2013): 1.843 1.73
Publication Forum (2013): 2
Scopus rating (2012): 1.644 1.591
Publication Forum (2012): 2
Hydrophobisation of wood surfaces by combining liquid flame spray (LFS) and plasma treatment: Dynamic wetting properties

The hydrophilic nature of wood surfaces is a major cause for water uptake and subsequent biological degradation and dimensional changes. In the present paper, a thin transparent superhydrophobic layer on pine veneer surfaces has been created for controlling surface wettability and water repellency. This effect was achieved by means of the liquid flame spray (LFS) technique, in the course of which the nanoparticulate titanium dioxide (TiO2) was brought to the surface, followed by plasma polymerisation. Plasma polymerised perfluorohexane (PFH)

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Organisations: Department of Physics, Research area: Aerosol Physics, Research group: Aerosol Synthesis, SP Technical Research Institute of Sweden, KTH, Royal Institute of Technology, Stockholm, Sweden
Authors: Moghammad, M. S., Heydari, G., Tuominen, M., Fielden, M., Haapanen, J., Mäkelä, J. M., Wålinder, M. E., Claesson, P. M., Swerin, A.
Keywords: (cold plasma, contact angle (CA), dynamic wetting, hexamethyldisiloxane (HMDSO), hydrophobisation, liquid flame spray (LFS), multi-scale roughness, nano-sized metal oxide (TiO2), perfluorohexane (PFH), plasma polymerisation, superhydrophobicity, Wilhelmy plate method, wood)
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Scopus rating (2015): 0.771 1.013
Web of Science (2015): 1.711 1.794 >10.0 0.414 0.00309 0.351
Publication Forum (2015): 1
Scopus rating (2014): 0.841 1.091
Web of Science (2014): 1.565 1.917 9.9 0.282 0.00343 0.374
Publication Forum (2014): 1
Scopus rating (2013): 0.89 1.295
Publication Forum (2013): 1
Interdigitation of long-chain sphingomyelin induces coupling of membrane leaflets in a cholesterol-dependent manner

It has been a long-standing question how the two leaflets in a lipid bilayer modulate each others' physical properties. In this paper, we discuss how this interaction may take place through interdigitation. We use atomistic molecular dynamics simulations to consider asymmetric lipid membrane models whose compositions are based on the lipidomics data determined for exosomes released by PC-3 prostate cancer cells. The simulations show interdigitation to be exceptionally strong for long-chain sphingomyelin (SM) molecules. In asymmetric membranes the amide-linked chain of SM is observed to extend deep into the opposing membrane leaflet. Interestingly, we find that the conformational order of the amide-linked SM chain increases the deeper it penetrates to the opposing leaflet. Analysis of this finding reveals that the amide-linked SM chain interacts favorably with the lipid chains in the opposite leaflet, and that cholesterol modulates the effect of SM interdigitation by influencing the conformational order of lipid hydrocarbon chains in the opposing (cytosolic) leaflet.

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Organisations: Department of Physics, Research area: Computational Physics, Research group: Biological Physics and Soft Matter, University of Limerick
Authors: Rog, T., Orlowski, A., Llorente, A., Skotland, T., Sylvanen, T., Kauhanen, D., Ekroos, K., Sandvig, K., Vattulainen, I.
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Web of Science (2015): 3.687 3.589 7.3 0.907 0.02731 1.163
Publication Forum (2015): 1
Scopus rating (2014): 1.869 1.09
Web of Science (2014): 3.836 3.881 7.0 1.006 0.02991 1.257
Publication Forum (2014): 2
Scopus rating (2013): 1.592 0.975
Publication Forum (2013): 2
Role of charged lipids in membrane structures: Insight given by simulations

Lipids and proteins are the main components of cell membranes. It is becoming increasingly clear that lipids, in addition to providing an environment for proteins to work in, are in many cases also able to modulate the structure and function of those proteins. Particularly charged lipids such as phosphatidylinositols and phosphatidylserines are involved in several examples of such effects. Molecular dynamics simulations have proved an invaluable tool in exploring these aspects. This so-called computational microscope can provide both complementing explanations for the experimental results and guide experiments to fruitful directions. In this paper, we review studies that have utilized molecular dynamics simulations to unravel the roles of charged lipids in membrane structures. We focus on lipids as active constituents of the membranes, affecting both general membrane properties as well as non-lipid membrane components, mainly proteins. This article is part of a Special Issue entitled: Biosimulations edited by Ilpo Vattulainen and Tomasz Róg.

General information

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Organisations: Department of Physics, Research area: Computational Physics, Research group: Biological Physics and Soft Matter, University of Helsinki, University of Southern Denmark
Authors: Pöyry, S., Vattulainen, I.
Keywords: (Cardiolipin, Lipid membrane, Lipid-protein interactions, Phosphatidylinositol, Phosphatidylserine)
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Publication Forum (2015): 1
Scopus rating (2014): 1.869 1.09
Web of Science (2014): 3.836 3.881 7.0 1.006 0.02991 1.257
Publication Forum (2014): 2
Scopus rating (2013): 1.592 0.975
Publication Forum (2013): 2
The biophysical properties of ethanolamine plasmalogens revealed by atomistic molecular dynamics simulations

Given the importance of plasmalogens in cellular membranes and neurodegenerative diseases, a better understanding of how plasmalogens affect the lipid membrane properties is needed. Here we carried out molecular dynamics simulations to study a lipid membrane comprised of ethanolamine plasmalogens (PE-plasmalogens). We compared the results to the PE-diacyl counterpart and palmitoyl-oleyl-phosphatidylcholine (POPC) bilayers. Results show that PE-plasmalogens form more compressed, thicker, and rigid lipid bilayers in comparison with the PE-diacyl and POPC membranes. The results also point out that the vinyl-ether linkage increases the ordering of sn-1 chain substantially and the ordering of the sn-2 chain to a minor extent. Further, the vinyl-ether linkage changes the orientation of the lipid head group, but it does not cause changes in the head group and glycerol backbone tilt angles with respect to the bilayer normal. The vinyl-ether linkage also packs the proximal regions of the sn-1 and sn-2 chains more closely together which also decreases the distance between the rest of the sn-1 and sn-2 chains.

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Organisations: Department of Physics, Research area: Computational Physics, Tampere University of Technology, VTT Technical Research Centre of Finland
Authors: Rog, T., Koivuniemi, A.
Keywords: Lipid membrane, Molecular dynamics, Neurodegenerative diseases, Plasmalogens
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Scopus rating (2015): 1.782 1.142
Web of Science (2015): 3.687 3.589 7.3 0.907 0.02731 1.163
Publication Forum (2015): 1
What can we learn about cholesterol's transmembrane distribution based on cholesterol-induced changes in membrane potential?

Cholesterol is abundant in the plasma membranes of animal cells and is known to regulate a variety of membrane properties. Despite decades of research, the transmembrane distribution of cholesterol is still a matter of debate. Here we consider this outstanding issue through atomistic simulations of asymmetric lipid membranes, whose composition is largely consistent with eukaryotic plasma membranes. We show that the membrane dipole potential changes in a cholesterol-dependent manner. Remarkably, moving cholesterol from the extracellular to the cytosolic leaflet increases the dipole potential on the cytosolic side, and vice versa. Biologically this implies that by altering the dipole potential, cholesterol can provide a driving force for cholesterol molecules to favor the cytosolic leaflet, in order to compensate for the intramembrane field that arises from the resting potential.

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Organisations: Department of Physics, Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Institute of Macromolecular Compounds, Russian Academy of Sciences, St. Petersburg, Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Flemingovo náměstí 542/2, 166 10 Praha 6, Czech Republic, Belozersky Institute of Physico-Chemical Biology, Lomonosov Moscow State University, Leninskie Gory, 1/40, 119991 Moscow, Russia
Authors: Falkovich, S. G., Martinez-Seara, H., Nesterenko, A. M., Vattulainen, I., Gurtovenko, A. A.
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Peer-reviewed: Yes

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ISSN (Print): 1948-7185
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Scopus rating (2016): 4.583 1.68
Mutually Exclusive Roles of SHARPIN in Integrin Inactivation and NF-κB Signaling

SHANK-associated RH domain interactor (SHARPIN) inhibits integrins through interaction with the integrin α-subunit. In addition, SHARPIN enhances nuclear factor-kappaB (NF-κB) activity as a component of the linear ubiquitin chain assembly complex (LUBAC). However, it is currently unclear how regulation of these seemingly different roles is coordinated. Here, we show that SHARPIN binds integrin and LUBAC in a mutually exclusive manner. We map the integrin binding site on SHARPIN to the ubiquitin-like (UBL) domain, the same domain implicated in SHARPIN interaction with LUBAC component RNF31 (ring finger protein 31), and identify two SHARPIN residues (V267, L276) required for both integrin and RNF31 regulation. Accordingly, the integrin α-tail is capable of competing with RNF31 for SHARPIN binding in vitro. Importantly, the full SHARPIN RNF31-binding site contains residues (F263A/I272A) that are dispensable for SHARPIN-integrin interaction. Importantly, disrupting SHARPIN interaction with integrin or RNF31 abolishes SHARPIN-mediated regulation of integrin or NF-κB activity, respectively. Altogether these data suggest that the roles of SHARPIN in inhibiting integrin activity and supporting linear ubiquitination are (molecularly) distinct.
Redox-induced activation of the proton pump in the respiratory complex I

Complex I functions as a redox-linked proton pump in the respiratory chains of mitochondria and bacteria, driven by the reduction of quinone (Q) by NADH. Remarkably, the distance between the Q reduction site and the most distant proton channels extends nearly 200 Å. To elucidate the molecular origin of this long-range coupling, we apply a combination of large-scale molecular simulations and a site-directed mutagenesis experiment of a key residue. In hybrid quantum mechanics/molecular mechanics simulations, we observe that reduction of Q is coupled to its local protonation by the His-38/Asp-139 ion pair and Tyr-87 of subunit Nqo4. Atomistic classical molecular dynamics simulations further suggest that formation of quinol (QH2) triggers rapid dissociation of the anionic Asp-139 toward the membrane domain that couples to conformational changes in a network of conserved charged residues. Site-directed mutagenesis data confirm the importance of Asp-139; upon mutation to asparagine the Q reductase activity is inhibited by 75%. The current results, together with earlier biochemical data, suggest that the proton pumping in complex I is activated by a unique combination of electrostatic and conformational transitions.

General information
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Organisations: Department of Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), Institute of Molecular Biotechnology, Jena, Germany, Technische Universität München, Institut für Informatik, Department of Theoretical Biophysics, Helsinki Bioenergetics Group Programme for Structural Biology and Biophysics, University of Helsinki Institute of Biotechnology, Max Planck Institute of Biophysics
Keywords: (Cell respiration, Electron transfer, Molecular dynamics simulations, NADH-quinone oxidoreductase, QM/MM simulations)
Number of pages: 6
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ASJC Scopus subject areas: General

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Publication Forum (2016): 3
Scopus rating (2015): 6.767 2.682
Scopus rating (2014): 6.853 2.725
Publication Forum (2014): 3
Scopus rating (2013): 6.989 2.73
Publication Forum (2013): 3
Scopus rating (2012): 6.792 2.682
Publication Forum (2012): 3
Scopus rating (2011): 6.771 2.636
Scopus rating (2010): 6.769 2.529
How To Minimize Artifacts in Atomistic Simulations of Membrane Proteins, Whose Crystal Structure Is Heavily Engineered: beta(2)-Adrenergic Receptor in the Spotlight

Atomistic molecular dynamics (MD) simulations are used extensively to elucidate membrane protein properties. These simulations are based on three-dimensional protein structures that in turn are often based on crystallography. The protein structures resolved in crystallographic studies typically do not correspond to pristine proteins, however. Instead the crystallized proteins are commonly engineered, including structural modifications (mutations, replacement of protein sequences by antibodies, bound ligands, etc.) whose impact on protein structure and dynamics is largely unknown. Here we explore this issue through atomistic MD simulations (~5 its in total), focusing on the beta(2)-adrenergic receptor (beta(2)AR) that is one of the most studied members of the G-protein coupled receptor superfamily. Starting from an inactive-state crystal structure beta(2)AR, we remove the many modifications in beta(2)AR systematically one at a time, in six consecutive steps. After each step, we equilibrate the system and simulate it quite extensively. The results of this step-by-step approach highlight that the structural modifications used in crystallization can affect ligand and G-protein binding sites, packing at the transmembrane-helix interface region, and the dynamics of connecting loops in beta(2)AR. When the results of the systematic step-by-step approach are compared to an all-at-once technique where all modifications done on beta(2)AR are removed instantaneously at the same time, it turns out that the step-by-step method provides results that are superior in terms of maintaining protein structural stability. The results provide compelling evidence that for membrane proteins whose 3D structure is based on structural engineering, the preparation of protein structure for atomistic MD simulations is a delicate and sensitive process. The results show that most valid results are found when the structural modifications are reverted slowly, one at a time.
Myelin protein P2 is a fatty acid-binding structural component of the myelin sheath in the peripheral nervous system, and its function is related to its membrane binding capacity. Here, the link between P2 protein dynamics and structure and function was studied using elastic incoherent neutron scattering (EINS). The P38G mutation, at the hinge between the β barrel and the α-helical lid, increased the lipid stacking capacity of human P2 in vitro, and the mutated protein was also functional in cultured cells. The P38G mutation did not change the overall structure of the protein. For a deeper insight into P2 structure-function relationships, information on protein dynamics in the 10 ps to 1 ns time scale was obtained using EINS. Values of mean square displacements mainly from protein H atoms were extracted for wild-type P2 and the P38G mutant and compared. Our results show that at physiological temperatures, the P38G mutant is more dynamic than the wild-type P2 protein, especially on a slow 1-ns time scale. Molecular dynamics simulations confirmed the enhanced dynamics of the mutant variant, especially within the portal region in the presence of bound fatty acid. The increased softness of the hinge mutant of human myelin P2 protein is likely related to an enhanced flexibility of the portal region of this fatty acid-binding protein, as well as to its interactions with the lipid bilayer surface requiring conformational adaptations.
Sec14-nodulin proteins and the patterning of phosphoinositide landmarks for developmental control of membrane morphogenesis

Polarized membrane morphogenesis is a fundamental activity of eukaryotic cells. This process is essential for the biology of cells and tissues, and its execution demands exquisite temporal coordination of functionally diverse membrane signaling reactions with high spatial resolution. Moreover, mechanisms must exist to establish and preserve such organization in the face of randomizing forces that would diffuse it. Here we identify the conserved AtSfh1 Sec14-nodulin protein as a novel effector of phosphoinositide signaling in the extreme polarized membrane growth program exhibited by growing Arabidopsis root hairs. The data are consistent with Sec14-nodulin proteins controlling the lateral organization of phosphatidylinositol 4,5-bisphosphate (PtdIns(4,5)P₂) landmarks for polarized membrane morphogenesis in plants. This patterning activity requires both the PtdIns(4,5)P₂ binding and homo-oligomerization activities of the AtSfh1 nodulin domain and is an essential aspect of the polarity signaling program in root hairs. Finally, the data suggest a general principle for how the phosphoinositide signaling landscape is physically bit mapped so that eukaryotic cells are able to convert a membrane surface into a high-definition lipid-signaling screen.
Role of subunit III and its lipids in the molecular mechanism of cytochrome c oxidase

The terminal respiratory enzyme cytochrome c oxidase (CcO) reduces molecular oxygen to water, and pumps protons across the inner mitochondrial membrane, or the plasma membrane of bacteria. A two-subunit CcO harbors all the elements necessary for oxygen reduction and proton pumping. However, it rapidly undergoes turnover-induced irreversible damage, which is effectively prevented by the presence of subunit III and its tightly bound lipids. We have performed classical atomistic molecular dynamics (MD) simulations on a three-subunit CcO, which show the formation of water wires between the polar head groups of lipid molecules bound to subunit III and the proton uptake site Asp91 (Bos taurus enzyme numbering). Continuum electrostatic calculations suggest that these lipids directly influence the proton affinity of Asp91 by 1-2 pK units. We surmise that lipids bound to subunit III influence the rate of proton uptake through the D-pathway, and therefore play a key role in preventing turnover-induced inactivation. Atomistic MD simulations show that subunit III is rapidly hydrated in the absence of internally bound lipids, which is likely to affect the rate of O$_2$ diffusion into the active-site. The role of subunit III with its indigenous lipids in the molecular mechanism of CcO is discussed.
The epidermal growth factor receptor (EGFR) regulates several critical cellular processes and is an important target for cancer therapy. In lieu of a crystallographic structure of the complete receptor, atomistic molecular dynamics (MD) simulations have recently shown that they can excel in studies of the full-length receptor. Here we present atomistic MD simulations of the monomeric N-glycosylated human EGFR in biomimetic lipid bilayers that are, in parallel, also used for the reconstitution of full-length receptors. This combination enabled us to experimentally validate our simulations, using...
ligand binding assays and antibodies to monitor the conformational properties of the receptor reconstituted into membranes. We find that N-glycosylation is a critical determinant of EGFR conformation, and specifically the orientation of the EGFR ectodomain relative to the membrane. In the absence of a structure for full-length, posttranslationally modified membrane receptors, our approach offers new means to structurally define and experimentally validate functional properties of cell surface receptors in biomimetic membrane environments.

**General information**

State: Published  
Ministry of Education publication type: A1 Journal article-refereed  
Organisations: Department of Physics, Tampere University of Technology, Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), University of Southern Denmark, Paul Langerhans Institute Dresden of the Helmholtz Centre Munich, University Clinic Carl Gustav Carus, TU Dresden, German Center for Diabetes Research (DZD e.V.), Max Planck Institute for Molecular Cell Biology and Genetics  
Authors: Kaszuba, K., Grzybek, M., Orłowski, A., Danne, R., Róg, T., Simons, K., Coskun, Ü., Vattulainen, I.  
Keywords: (EGFR, Lipid-protein interaction, Lipids, MD simulation, Proteoliposomes)  
Number of pages: 6  
Pages: 4334-4339  
Publication date: 7 Apr 2015  
Peer-reviewed: Yes  
ASJC Scopus subject areas: General

**Publication information**

Journal: Proceedings of the National Academy of Sciences of the United States of America  
Volume: 112  
Issue number: 14  
ISSN (Print): 0027-8424  
Ratings:  
Publication Forum (2017): 3  
Publication Forum (2016): 3  
Scopus rating (2015): 6.767 2.682  
Scopus rating (2014): 6.853 2.725  
Publication Forum (2014): 3  
Scopus rating (2013): 6.989 2.73  
Publication Forum (2013): 3  
Scopus rating (2012): 6.792 2.682  
Publication Forum (2012): 3  
Scopus rating (2011): 6.771 2.636  
Scopus rating (2010): 6.769 2.529  
Scopus rating (2007): 6.766 2.441  
Scopus rating (2005): 6.784 2.551  
Scopus rating (2004): 7.026 2.622  
Scopus rating (2003): 7.018 2.501  
Scopus rating (2001): 7.192 2.463  
Scopus rating (2000): 7.731 2.475  
Scopus rating (1999): 8.271 2.446  
Original language: English  
DOIs: 10.1073/pnas.1503262112  
Links: http://www.scopus.com/inward/record.url?scp=84929500864&partnerID=8YFLogxK (Link to publication in Scopus)

**Bibliographical note**
Oxidation of cholesterol does not alter significantly its uptake into high-density lipoprotein particles

Using replica exchange umbrella sampling we calculated free energy profiles for uptake of cholesterol and one of its oxysterols (7-ketocholesterol) from an aqueous solution into a high-density lipoprotein particle. These atomistic molecular dynamics simulations show that both sterols are readily taken up from the aqueous solution with comparable free energy minima at the surface of the particle of -17 kcal/mol for cholesterol and -14 kcal/mol for 7-ketocholesterol. Moreover, given its preferred position at the particle surface, 7-ketocholesterol is expected to be able to participate directly in biological signaling processes.

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Department of Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), University of Southern Denmark, Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
Authors: Karilainen, T., Timr, Š., Vattulainen, I., Jungwirth, P.
Number of pages: 7
Pages: 4594-4600
Publication date: 2 Apr 2015
Peer-reviewed: Yes
ASJC Scopus subject areas: Physical and Theoretical Chemistry, Materials Chemistry, Surfaces, Coatings and Films

Publication information
Journal: Journal of Physical Chemistry Part B
Volume: 119
Issue number: 13
ISSN (Print): 1520-6106
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.348 1.02
Publication Forum (2016): 1
Scopus rating (2015): 1.367 1.096
Web of Science (2015): 3.187 3.265 9.8 0.808 0.11793 0.91
Publication Forum (2015): 1
Scopus rating (2014): 1.44 1.14
Web of Science (2014): 3.302 3.528 9.0 0.754 0.14274 0.989
Publication Forum (2014): 3
Scopus rating (2013): 1.494 1.2
Publication Forum (2013): 3
Scopus rating (2012): 1.92 1.251
Publication Forum (2012): 3
Scopus rating (2011): 1.78 1.226
Scopus rating (2010): 1.849 1.214
Scopus rating (2009): 2.232 1.349
Scopus rating (2008): 2.543 1.381
Scopus rating (2007): 2.346 1.282
Scopus rating (2006): 2.369 1.415
Scopus rating (2005): 2.275 1.474
Scopus rating (2004): 2.148 1.511
Scopus rating (2003): 2.034 1.47
Scopus rating (2002): 2.118 1.496
Scopus rating (2001): 2.053 1.508
Scopus rating (2000): 2.145 1.527
Scopus rating (1999): 1.713 1.8
Original language: English
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.
Experimental determination and computational interpretation of biophysical properties of lipid bilayers enriched by cholesteryl hemisuccinate

Cholesteryl hemisuccinate (CHS) is one of the cholesterol-mimicking detergents not observed in nature. It is, however, widely used in protein crystallography, in biochemical studies of proteins, and in pharmacology. Here, we performed an extensive experimental and theoretical study on the behavior of CHS in lipid membranes rich in unsaturated phospholipids. We found that the deprotonated form of CHS (that is the predominant form under physiological conditions) does not mimic cholesterol very well. The protonated form of CHS does better in this regard, but also its ability to mimic the physical effects of cholesterol on lipid membranes is limited. Overall, although ordering and condensing effects characteristic to cholesterol are present in systems containing any form of CHS, their strength is appreciably weaker compared to cholesterol. Based on the considerable amount of experimental and atomistic simulation data, we conclude that these differences originate from the fact that the ester group of CHS does not anchor it in an optimal position at the water-membrane interface. The implications of these findings for considerations of protein-cholesterol interactions are briefly discussed.

General information

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Organisations: Department of Physics, Research group: Biological Physics and Soft Matter, Computational Science X (CompX), Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, University of Southern Denmark
Authors: Kulig, W., Jurkiewicz, P., Olzyńska, A., Tynkkynen, J., Javanainen, M., Manna, M., Rog, T., Hof, M., Vattulainen, I., Jungwirth, P.
Keywords: (Cholesterol-mimicking detergents, DPH, Dynamic light scattering, Laurdan, Molecular dynamics simulations, Time-dependent fluorescence shift)
Number of pages: 11
Pages: 422-432
Publication date: 2015
Peer-reviewed: Yes
Early online date: 25 Oct 2014
ASJC Scopus subject areas: Biochemistry, Cell Biology, Biophysics, Medicine(all)

Publication information
Journal: Biochimica et Biophysica Acta: Biomembranes
Volume: 1848
Issue number: 2
ISSN (Print): 0005-2736
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.511 1.101
Publication Forum (2016): 1
Scopus rating (2015): 1.782 1.142
Web of Science (2015): 3.687 3.589 7.3 0.907 0.02731 1.163
Publication Forum (2015): 1
Scopus rating (2014): 1.869 1.09
How endoglucanase enzymes act on cellulose nanofibrils: role of amorphous regions revealed by atomistic simulations

Transformation of cellulose into monosaccharides can be achieved in a chemical process performed by a special group of enzymes known as cellulases. We have used atomistic molecular dynamics simulations to study endoglucanase II (Cel5A) that is one of the proteins in this group. Based on the atomistic simulation results, we discuss how the Cel5A enzyme interacts with cellulose fibrils comprised of both crystalline and amorphous regions. We show that the enzyme’s carbohydrate-binding domain prefers to interact with crystalline regions of cellulose, while the catalytic domain has a high affinity to the amorphous regions of fibrils. In particular, through electrostatic interactions the catalytic domain attracts loose glucose chains to its catalytic cleft. The atomistic details of the enzyme–cellulose interaction are presented and the implications for practical applications are briefly discussed.
How mono-valent cations bend peptide turns and a first-principles database of amino acids and dipeptides

In this contribution we detail our efforts to investigate the structural effects of cations binding to peptides and amino acids. We perform first-principles studies employing long-range dispersion-corrected approximate density-functional theory and compare to gas-phase experiments.

**General information**

State: Published

Ministry of Education publication type: A4 Article in a conference publication

Organisations: Department of Physics, Research area: Computational Physics, Computational Science X (CompX), Fritz Haber Institute of the Max Planck Society, COMP Centre of Excellence, Department of Applied Physics, Aalto University, Duke University

Authors: Baldauf, C., Ropo, M., Blum, V., Scheffler, M.

Keywords: (benchmarks, conformation database, density-functional theory, Peptide conformation, theoretical vibrational spectroscopy)

Number of pages: 2

Pages: 119-120

Publication date: 6 Oct 2014

**Host publication information**

Title of host publication: International Conference of Computational Methods in Sciences and Engineering 2014 (ICCMSE 2014)
Membrane-associated proteins do care about lipids - perspective based on atomistic molecular dynamics simulations

This thesis consists of three original articles that deal with lipid-protein interactions investigated using atomistic molecular dynamics simulations method, which in some cases were complemented with experimental data. Since very few molecular details of these important interactions are known, the data shown in this thesis can help to understand and develop a broader view on the role of lipids in protein's function. In the first part of this thesis, the membrane-binding part of the COMT protein was studied using the atomistic molecular dynamics simulations. The results indicate that the role of the transmembrane helix and the linker part of this protein is to enclose the enzymatic part of the protein in the close vicinity of the membrane, and therefore to keep it in the specific membrane-water interface environment. Moreover, the particular kind of protein fold, which includes a specific salt bridge in the linker part of the protein, was found in almost all of the simulations, and this information was evaluated further to reveal that this can be the general folding motif for all similar proteins that possess one transmembrane helix and a short linker part that joins it with the rest of the protein. By continuation of the urge to explain the role of the membrane in enzymatic function of COMT, another idea was also investigated: namely, the suggestion that ligands for that enzyme might have different characteristics in regard to their affinity to how the membrane was evaluated, to check whether the membrane binding part of COMT role is indeed meant to make it more accessible to those ligands which stay close to the membrane. This idea was studied with the atomistic molecular dynamics simulations where two COMT ligands—dopamine and L-dopa—were simulated with the membranes of various compositions, and furthermore the results were validated by experiments. The data from that study was consistent with the suggested idea of preferential binding of some ligands to lipids, but also this finding has been shown to have more possible implications for the neurotransmission process and other highly important physiological processes.

The second part of this work focuses on the role of cholesterol in hydrophobic matching of peptides and the resulting sorting of transmembrane peptides according to their hydrophobic length. Experimental data from collaborating team suggested that under negative mismatch and the presence of cholesterol in membranes, peptides could laterally sort. Nevertheless, molecular mechanisms of that were unclear. Atomistic molecular dynamics simulations performed for this part of the thesis revealed that cholesterol increases the significance of the negative hydrophobic mismatch, and thus it shifts preference of proteins in such conditions to cluster into domains to minimize the mismatch. In the second part of this study, extended atomistic molecular dynamics simulations showed that cholesterol has a preference to stay in the vicinity of the peptide under negative mismatch when compared to a positive mismatch case. Even more strikingly, cholesterol orients around the negatively mismatched peptide in a special geometrical configuration with its rough side exposed in the direction of peptide. In summation, studies for this work demonstrated a view on some aspects of the lipid-protein interactions at the molecular level retrieved through the atomistic molecular dynamics simulations. Importantly, many of the aspects presented here were validated with experiments or suggested explanation for the phenomena observed beforehand by experimental methods. Certainly, lipids are important for the function of proteins, and as it is shown in this thesis, joining experimental and computational approach is a very good way to understand this complicated interplay better and to provide atomistic details of these dynamic processes.
Computational Modeling of Functional Gold Nanoparticles in Biological Environment

This work focuses on exploring the properties and functions of charged monolayer-protected gold nanoparticles (AuNPs) in biologically relevant environments by use of atomic-scale molecular dynamics (MD) simulations.

The use of nanoparticles (NPs) in modern technology has been increasing rapidly during the last few years. NPs of different kinds have already been employed, e.g., in nanomedicine as cancer treatments, cleaning agents, cosmetics and new materials for industrial purposes. AuNPs are one type of nanoagents that are being employed for such purposes, and according to recent experimental findings they may have cytotoxic properties. In particular, AuNPs of 2-nm diameter or less are known to permeate through plasma membranes and induce cell death. Hence, studying potential harmful effects of AuNPs is of importance. Understanding the interaction between NPs and cell membranes is relevant also because all trafficking between the cell interior and extracellular space takes place through the cell membrane.

The first study concentrated on the properties of AuNPs in aqueous solution at physiological temperature (310 K). The results showed that electrostatic properties modulate the formation of a complex comprised of the AuNP together with surrounding ions and water, and suggested that electrostatics is one of the central factors in the complexation of AuNPs with other nanomaterials and biological systems. The results highlighted the importance of long-range electrostatic interactions in determining NP properties in aqueous solutions. This observation was concluded to indicate an important role in the interplay between NPs and lipid membranes, which surround cells.

The second part of the research comprises of studying AuNPs in the presence of model cell membranes. The binding of AuNP and membrane reorganization processes were discovered to be governed by co-operative effects where AuNP, counter ions, water and membrane all contribute. The results suggest that a permeation of a cationic AuNP takes place through pore-formation with partial NP neutralization, leading to membrane disruption at higher NP concentrations. The results also suggested a potential mechanism for cytotoxicity as cationic AuNP binding to the extracellular leaflet may trigger apoptosis through translocation of phosphatidylserine.

Summa summarum, the work presented here provides novel aspects on the interactions of functional AuNPs on cellular level by means of atomistic MD simulation.
Electronic versions:
heikkila.pdf
Links:

Bibliographical note
Awarding institution: Tampere University of Technology
Source: researchoutputwizard
Source-ID: 422
Research output: Collection of articles › Doctoral Thesis

Atomistic Molecular Dynamics Simulations of Cytochrome bc1, and Epiderm Growth Factor Receptor Proteins

General information
State: Published
Ministry of Education publication type: G4 Doctoral dissertation (monograph)
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Kaszuba, K.
Publication date: 2014

Publication information
Publisher: Tampere University of Technology
Original language: English

Publication series
Name: Tampere University of Technology, Publication
Publisher: Tampere University of Technology
Volume: 1271
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Bibliographical note
Awarding institution: Tampere University of Technology
Source: researchoutputwizard
Source-ID: 676
Research output: Monograph › Doctoral Thesis

Atomistic simulations of anionic Au144(SR)60 nanoparticles interacting with asymmetric model lipid membranes

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Research group: Materials and Molecular Modeling, Department of Physics, Computational Science X (CompX)
Authors: Heikkilä, E., Martinez-Seara, H., Gurtovenko, A. A., Vattulainen, I., Akola, J.
Number of pages: 9
Pages: 2852-2860
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Biochimica et Biophysica Acta: Biomembranes
Volume: 1838
Issue number: 11
ISSN (Print): 0005-2736
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.511 1.101
Publication Forum (2016): 1
Scopus rating (2015): 1.782 1.142
Web of Science (2015): 3.687 3.589 7.3 0.907 0.02731 1.163
Publication Forum (2015): 1
Cationic Au Nanoparticle Binding with Plasma Membrane-like Lipid Bilayers: Potential Mechanism for Spontaneous Permeation to Cells Revealed by Atomistic Simulations

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Research group: Materials and Molecular Modeling, Department of Physics, Computational Science X (CompX)
Authors: Heikkilä, E., Martinez-Seara, H., Gurtovenko, A. A., Javanainen, M., Häkkinen, H., Vattulainen, I., Akola, J.
Number of pages: 11
Pages: 11131-11141
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 118
Issue number: 20
ISSN (Print): 1932-7447
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.948 1.181
Publication Forum (2016): 1
Scopus rating (2015): 1.917 1.268
Web of Science (2015): 4.509 4.919 4.7 0.829 0.28449 1.171
Publication Forum (2015): 1
Scopus rating (2014): 2.027 1.448
Web of Science (2014): 4.772 5.295 4.3 0.768 0.30727 1.234
Cholesterol level affects surface charge of lipid membranes in saline solution

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX)
Authors: Magarkar, A., Dhawan, V., Kallilnteri, P., Viitala, T., Elmowafy, M., Rog, T., Bunker, A.
Number of pages: 5
Pages: 1-5
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Scientific Reports
Volume: 4
Article number: 5005
ISSN (Print): 2045-2322
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.625 1.401
Publication Forum (2016): 2
Scopus rating (2015): 2.057 1.684
Web of Science (2015): 5.228 5.525 2.1 0.559 0.20942 1.865
Publication Forum (2015): 2
Scopus rating (2014): 2.103 1.544
Web of Science (2014): 5.578 5.597 1.7 0.722 0.11476 2.075
Publication Forum (2014): 1
Scopus rating (2013): 1.886 1.51
Publication Forum (2013): 1
Scopus rating (2012): 1.458 0.896
Publication Forum (2012): 1
Original language: English
DOIs:
10.1038/srep05005

Bibliographical note
Contribution: organisation=fys,FACT1=1<br/>Portfolio EDEND: 2014-09-30<br/>Publisher name: Nature Publishing Group
Source: researchoutputwizard
Source-ID: 985
Cholesterol, sphingolipids and glycolipids: What do we know about their role in raft-like membranes?

**General information**
State: Published
Ministry of Education publication type: A2 Review article in a scientific journal
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX)
Authors: Rog, T., Vattulainen, I.
Number of pages: 22
Pages: 82-104
Publication date: 2014
Peer-reviewed: Yes

**Publication information**
Journal: Chemistry and Physics of Lipids
Volume: 184
ISSN (Print): 0009-3084
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.976 0.862
Publication Forum (2016): 1
Scopus rating (2015): 0.957 0.957
Web of Science (2015): 2.901 2.75 >10.0 0.868 0.00491 0.736
Publication Forum (2015): 1
Scopus rating (2014): 0.885 1.039
Web of Science (2014): 2.422 2.697 >10.0 1.233 0.00529 0.788
Publication Forum (2014): 1
Scopus rating (2013): 0.82 1.055
Publication Forum (2013): 1
Scopus rating (2012): 0.803 0.974
Publication Forum (2012): 1
Scopus rating (2011): 0.727 0.984
Scopus rating (2010): 0.874 0.964
Scopus rating (2009): 0.9 0.995
Scopus rating (2008): 1.114 1.057
Scopus rating (2007): 1.083 1.091
Scopus rating (2006): 0.808 0.881
Scopus rating (2005): 1.038 1.035
Scopus rating (2004): 0.69 0.831
Scopus rating (2003): 0.917 0.817
Scopus rating (2002): 1.005 0.813
Scopus rating (2001): 1.097 0.827
Scopus rating (2000): 0.738 0.742
Scopus rating (1999): 0.737 0.705
Original language: English
DOIs:
10.1016/j.chemphyslip.2014.10.004

**Bibliographical note**
Contribution: organisation=fys,FACT1=1<br/>Portfolio EDEND: 2014-12-15<br/>Publisher name: Elsevier Ireland Ltd
Source: researchoutputwizard
Source-ID: 1391
Research output: Scientific - peer-review › Review Article
Co-exposure with fullerene may strengthen health effects of organic industrial chemicals

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX), Multi-scaled biodata analysis and modelling (MultiBAM)
Authors: Lehto, M., Karilainen, T., Rog, T., Cramariuc, O., Vanhala, E., Yrnnaeus, J., Taberman, H., Jänis, J., Alenius, H., Vattulainen, I., Laine, O.
Number of pages: 24
Pages: 1-24
Publication date: 2014
Peer-reviewed: Yes

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Journal: PLoS One
Volume: 9
Issue number: 12
Article number: e114490
ISSN (Print): 1932-6203
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.201 1.092
Scopus rating (2015): 1.414 1.131
Web of Science (2015): 3.057 3.535 3.1 0.396 1.81924 1.139
Publication Forum (2015): 1
Scopus rating (2014): 1.545 1.141
Web of Science (2014): 3.234 3.702 2.7 0.489 1.53341 1.209
Publication Forum (2014): 2
Scopus rating (2013): 1.74 1.147
Publication Forum (2013): 2
Scopus rating (2012): 1.945 1.142
Publication Forum (2012): 2
Scopus rating (2011): 2.369 1.23
Scopus rating (2010): 2.631 1.161
Scopus rating (2009): 2.473 0.985
Scopus rating (2008): 2.323 0.96
Scopus rating (2007): 1.289 0.525
Original language: English
DOIs:
10.1371/journal.pone.0114490

Bibliographical note
Contribution: organisation=fys,FACT1=1<br/>Portfolio EDEND: 2014-12-15<br/>Publisher name: Public Library of Science
Source: researchoutputwizard
Source-ID: 908
Research output: Scientific - peer-review › Article

Collective dynamics effect transient subdiffusion of inert tracers in flexible gel networks

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Godec, A., Bauer, M., Metzler, R.
Number of pages: 13
Pages: 1-13
Publication date: 2014
Peer-reviewed: Yes
Critical adsorption of polyelectrolytes onto charged Janus nanospheres

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: de Carvalho, S. J., Metzler, R., Cherstvy, A. G.
Number of pages: 12
Pages: 15539-15550
Publication date: 2014
Peer-reviewed: Yes
Deformation propagation in responsive polymer network films

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Ghosh, S. K., Cherstvy, A. G., Metzler, R.
Number of pages: 10
Pages: 1-9
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Physics
Volume: 141
Issue number: 7
Article number: 074903
ISSN (Print): 0021-9606
Ratings:
Dehydroergosterol as an Analogue for Cholesterol: Why It Mimics Cholesterol So Well - or Does It?

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX), Multi-scaled biodata analysis and modelling (MultiBAM)
Authors: Pourmousa, M., Rog, T., Mikkeli, R., Vattulainen, I., Solanko, L. M., Wustner, D., Holmgaard List, N., Kongsted, J., Karttunen, M.
Number of pages: 13
Pages: 7345-7357
Publication date: 2014
Peer-reviewed: Yes

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Journal: Journal of Physical Chemistry Part B
Volume: 118
Issue number: 26
ISSN (Print): 1520-6106
Ratings:

Publication Forum (2017): 1
Scopus rating (2016): 1.073 0.755
Publication Forum (2016): 1
Scopus rating (2015): 0.953 0.767
Web of Science (2015): 2.894 2.95 >10.0 0.786 0.16944 0.873
Publication Forum (2015): 1
Scopus rating (2014): 1.386 0.989
Web of Science (2014): 2.952 3.017 >10.0 0.731 0.18296 0.916
Publication Forum (2014): 3
Scopus rating (2013): 1.532 1.17
Publication Forum (2013): 3
Scopus rating (2012): 1.787 1.118
Publication Forum (2012): 3
Scopus rating (2011): 1.805 1.207
Scopus rating (2010): 1.73 1.052
Scopus rating (2009): 2.003 1.104
Scopus rating (2008): 2.189 1.12
Scopus rating (2007): 2.163 1.108
Scopus rating (2006): 2.176 1.266
Scopus rating (2005): 2.27 1.359
Scopus rating (2004): 2.229 1.369
Scopus rating (2003): 2.121 1.322
Scopus rating (2002): 2.256 1.341
Scopus rating (2001): 2.381 1.362
Scopus rating (2000): 2.576 1.423
Scopus rating (1999): 2.133 1.419
Original language: English
DOIs:
10.1063/1.4893056

Bibliographical note
Contribution: organisation=fys,FACT1=1<br/>Portfolio EDEND: 2014-12-04<br/>Publisher name: American Institute of Physics
Source: researchoutputwizard
Source-ID: 342
Research output: Scientific - peer-review > Article
Enzymatic oxidation of cholesterol: Properties and functional effects of cholestenone in cell membranes

General information
State: Published
Ministry of Education publication type: A1 Journal article-referred
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX)
Authors: Neuvonen, M., Manna, M., Mokkila, S., Javanainen, M., Rog, T., Liu, Z., Bittman, R., Vattulainen, I., Ikonen, E.
Number of pages: 13
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: PLoS One
Volume: 9
Issue number: 8
Article number: e103743
ISSN (Print): 1932-6203
Ratings:

Scopus rating (2016): 1.348 1.02
Publication Forum (2016): 1
Scopus rating (2015): 1.367 1.096
Web of Science (2015): 3.187 3.265 9.8 0.808 0.11793 0.91
Publication Forum (2015): 1
Scopus rating (2014): 1.44 1.14
Web of Science (2014): 3.302 3.528 9.0 0.754 0.14274 0.989
Publication Forum (2014): 3
Scopus rating (2013): 1.494 1.2
Publication Forum (2013): 3
Scopus rating (2012): 1.92 1.251
Publication Forum (2012): 3
Scopus rating (2011): 1.78 1.226
Scopus rating (2010): 1.849 1.214
Scopus rating (2009): 2.232 1.349
Scopus rating (2008): 2.543 1.381
Scopus rating (2007): 2.346 1.282
Scopus rating (2006): 2.369 1.415
Scopus rating (2005): 2.275 1.474
Scopus rating (2004): 2.148 1.511
Scopus rating (2003): 2.034 1.47
Scopus rating (2002): 2.118 1.496
Scopus rating (2001): 2.053 1.508
Scopus rating (2000): 2.145 1.527
Scopus rating (1999): 1.713 1.8
Original language: English
DOI: 10.1021/jp406883k
First-passage statistics for aging diffusion in systems with annealed and quenched disorder

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Krusemann, H., Godec, A., Metzler, R.
Number of pages: 5
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Physical Review E
Volume: 89
Issue number: 4
Article number: 040101
ISSN (Print): 1539-3755

Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 0.993 0.896
Publication Forum (2016): 1
Scopus rating (2015): 1.047 0.978
Publication Forum (2015): 1
Scopus rating (2014): 1.22 1.123
Web of Science (2014): 2.288 2.269 8.5 0.595 0.16687 0.859
Publication Forum (2014): 2
Scopus rating (2013): 1.311 1.239
Publication Forum (2013): 2
Scopus rating (2012): 1.42 1.226
Publication Forum (2012): 2
Scopus rating (2011): 1.485 1.225
How Anacetrapib Inhibits the Activity of the Cholesteryl Ester Transfer Protein? Perspective through Atomistic Simulations

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX)
Authors: Äijänen, T., Koivuniemi, A., Javanainen, M., Rissanen, S., Rog, T., Vattulainen, I.
Number of pages: 14
Pages: 1-14
Publication date: 2014
Peer-reviewed: Yes

Publication Information
Journal: PLOS Computational Biology
Volume: 10
Issue number: 11
Article number: e1003987
ISSN (Print): 1553-7358
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 3.144 1.342
Publication Forum (2016): 2
Scopus rating (2015): 3.43 1.447
Web of Science (2015): 4.587 5.017 4.5 0.568 0.085 46 2.349
Publication Forum (2015): 2
Scopus rating (2014): 3.359 1.44
Web of Science (2014): 4.62 5.279 4.3 0.807 0.082 4 2.339
Publication Forum (2014): 3
Scopus rating (2013): 3.295 1.457
Publication Forum (2013): 3
Scopus rating (2012): 3.329 1.642
Publication Forum (2012): 3
Scopus rating (2011): 3.381 1.603
Scopus rating (2010): 3.523 1.554
Scopus rating (2009): 3.273 1.44
Scopus rating (2007): 3.09 1.264
Scopus rating (2006): 1.988 1.018
Original language: English
DOIs: 10.1371/journal.pcbi.1003987

Bibliographical note
Contribution: organisation=fys,FAC1=1<br/>Portfolio EDEND: 2014-12-16<br/>Publisher name: Public Library of Science; International Society for Computational Biology
Source: researchoutputwizard
Source-ID: 72
Research output: Scientific - peer-review Article

Mixing and segregation of ring polymers: spatial confinement and molecular crowding effects

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Shin, J., Cherstvy, A., Metzler, R.
Number of pages: 19
Pages: 1-19
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: New Journal of Physics
Volume: 16
Article number: 053047
ISSN (Print): 1367-2630
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.788 1.031
Publication Forum (2016): 2
Scopus rating (2015): 1.938 1.047
Web of Science (2015): 3.57 3.501 4.7 1.118 0.10691 1.706
Publication Forum (2015): 2
Scopus rating (2014): 2.806 1.307
Web of Science (2014): 3.558 3.664 4.4 0.861 0.12987 1.982
Publication Forum (2014): 2
Scopus rating (2013): 2.871 1.372
Publication Forum (2013): 2
Scopus rating (2012): 3.352 1.533
Publication Forum (2012): 2
Scopus rating (2011): 3.47 1.634
Scopus rating (2010): 3.395 1.421
Scopus rating (2008): 2.913 1.396
Scopus rating (2007): 2.825 1.354
Scopus rating (2006): 2.2 1.296
Scopus rating (2005): 1.641 1.116
Scopus rating (2004): 1.211 1.009
Scopus rating (2003): 1.057 0.75
Scopus rating (2002): 0.77 0.666
Scopus rating (2001): 1.033 0.843
Molecular Dynamics Simulation of Inverse-Phosphocholine Lipids

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX)
Authors: Magarkar, A., Rog, T., Bunker, A.
Number of pages: 6
Pages: 19444-19449
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Physical Chemistry C
Volume: 118
Issue number: 33
ISSN (Print): 1932-7447
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.948 1.181
Publication Forum (2016): 1
Scopus rating (2015): 1.917 1.268
Web of Science (2015): 4.509 4.919 4.7 0.829 0.28449 1.171
Publication Forum (2015): 1
Scopus rating (2014): 2.027 1.448
Web of Science (2014): 4.772 5.295 4.3 0.768 0.307 1.234
Publication Forum (2014): 3
Scopus rating (2013): 2.134 1.439
Publication Forum (2013): 3
Scopus rating (2012): 2.514 1.46
Publication Forum (2012): 3
Scopus rating (2011): 2.32 1.457
Scopus rating (2010): 2.438 1.356
Scopus rating (2009): 2.128 1.417
Scopus rating (2008): 1.856 1.033
Original language: English
DOIs:
10.1021/jp505633y

Bibliographical note
Contribution: organisation=fys,FACT1=1<br/>Portfolio EDEND: 2014-12-18<br/>Publisher name: Institute of Physics Publishing Ltd.; Deutsche Physikalische Gesellschaft
Source: researchoutputwizard
Source-ID: 1494
Research output: Scientific - peer-review › Article
Nonergodicity, fluctuations, and criticality in heterogeneous diffusion processes

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Cherstvy, A., Metzler, R.
Number of pages: 12
Pages: 1-12
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Physical Review E
Volume: 90
Nonlinear multipolar light-matter interactions with gaussian vector beams

General information
State: Published
Ministry of Education publication type: B3 Non-refereed article in conference proceedings
Organisations: Research group: Nonlinear Optics, Research area: Optics, Department of Physics
Authors: Huttunen, M., Mäkitalo, J., Bautista, G., Kauranen, M.
Number of pages: 1
Pages: 8-8
Publication date: 2014

Host publication information
Editor: Saarinen, J. J.

Bibliographical note
Contribution: organisation=fys,FACT1=1<br/>Portfolio EDEND: 2014-12-17
Source: researchoutputwizard
Source-ID: 222
Research output: Scientific - peer-review › Article
Polymer translocation: the first two decades and the recent diversification

General information
State: Published
Ministry of Education publication type: A2 Review article in a scientific journal
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Palyulin, V. V., Ala-Nissilä, T., Metzler, R.
Pages: 9016-9037
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Soft Matter
Volume: 10
Issue number: 45
ISSN (Print): 1744-683X
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.573 1.219
Publication Forum (2016): 2
Scopus rating (2015): 1.67 1.33
Web of Science (2015): 3.798 4.001 4.0 0.949 0.10203 1.206
Publication Forum (2015): 2
Scopus rating (2014): 1.751 1.267
Web of Science (2014): 4.029 4.289 3.4 1.105 0.10152 1.227
Publication Forum (2014): 3
Scopus rating (2013): 1.745 1.208
Publication Forum (2013): 3
Scopus rating (2012): 1.898 1.155
Publication Forum (2012): 3
Scopus rating (2011): 2.006 1.314
Scopus rating (2010): 2.165 1.376
Scopus rating (2009): 2.516 1.534
Scopus rating (2008): 2.562 1.392
Scopus rating (2007): 2.482 1.458
Scopus rating (2006): 1.899 0.981
Original language: English
DOIs:
10.1039/c4sm01819b

Bibliographical note
Contribution: organisation=fys,FACT1=1<br/>Portfolio EDEND: 2014-12-17<br/>Publisher name: R S C Publications
Source: researchoutputwizard
Source-ID: 1226
Research output: Scientific - peer-review › Review Article

Refined OPLS All-Atom Force Field for Saturated Phosphatidylcholine Bilayers at Full Hydration

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX), Multi-scaled biodata analysis and modelling (MultiBAM)
Authors: Maciejewski, A., Pasenkiewicz-Gierula, M., Cramariuc, O., Vattulainen, I., Rog, T.
Number of pages: 11
Pages: 4571-4581
Publication date: 2014
Peer-reviewed: Yes
Scaled Brownian motion: a paradoxical process with a time dependent diffusivity for the description of anomalous diffusion

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Jeon, J., Chechkin, A. V., Metzler, R.
Number of pages: 7
Pages: 15811-15817
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 16
Issue number: 30
ISSN (Print): 1463-9076
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 1.678 1.117
Publication Forum (2016): 1
Scopus rating (2015): 1.771 1.244
Web of Science (2015): 4.449 4.273 4.1 1.017 0.19255 1.158
Publication Forum (2015): 1
Single Lipid Extraction: The Anchoring Strength of Cholesterol in Liquid-Ordered and Liquid-Disordered Phases

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX)
Authors: Stetter, F., Cwiklic, L., Jungwirth, P., Hugel, T.
Number of pages: 9
Pages: 1167-1175
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Biophysical Journal
Volume: 107
Issue number: 5
ISSN (Print): 0006-3495
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 1.946 1.018
Publication Forum (2016): 2
Scopus rating (2015): 2.145 1.173
Web of Science (2015): 3.632 3.668 >10.0 0.919 0.07519 1.522
Publication Forum (2015): 2
Scopus rating (2014): 2.203 1.166
Web of Science (2014): 3.972 3.874 9.6 0.924 0.08587 1.538
Publication Forum (2014): 3
The challenges of understanding glycolipid functions: An open outlook based on molecular simulations

General information
State: Published
Ministry of Education publication type: A2 Review article in a scientific journal
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics, Computational Science X (CompX)
Authors: Manna, M., Rog, T., Vattulainen, I.
Number of pages: 16
Pages: 1130-1145
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Biochimica et Biophysica Acta: Molecular and Cell Biology of Lipids
Volume: 1841
Issue number: 8
ISSN (Print): 1388-1981
Ratings:
Publication Forum (2017): 1
Scopus rating (2016): 2.59 1.445
Publication Forum (2016): 1
Scopus rating (2015): 2.53 1.316
Web of Science (2015): 4.779 4.541 5.8 1.993 0.01842 1.523
Publication Forum (2015): 1
Scopus rating (2014): 2.408 1.282
Web of Science (2014): 5.162 4.904 5.6 1.265 0.02062 1.711
Publication Forum (2014): 2
Scopus rating (2013): 2.181 1.313
Publication Forum (2013): 2
Scopus rating (2012): 2.17 1.297
Universal Method for Embedding Proteins into Complex Lipid Bilayers for Molecular Dynamics Simulations

General information
State: Published
Ministry of Education publication type: A1 Journal article-refereed
Organisations: Research area: Computational Physics, Research group: Biological Physics and Soft Matter, Department of Physics
Authors: Javanainen, M.
Number of pages: 6
Pages: 2577-2582
Publication date: 2014
Peer-reviewed: Yes

Publication information
Journal: Journal of Chemical Theory and Computation
Volume: 10
Issue number: 6
ISSN (Print): 1549-9618
Ratings:
Publication Forum (2017): 2
Scopus rating (2016): 2.801 1.589
Publication Forum (2016): 2
Scopus rating (2015): 2.795 1.748
Web of Science (2015): 5.301 5.756 4.3 1.134 0.0635 1.768
Publication Forum (2015): 2
Scopus rating (2014): 2.777 1.603
Web of Science (2014): 5.498 5.76 3.9 1.195 0.05994 1.761
Publication Forum (2014): 2
Scopus rating (2013): 2.409 1.578
Publication Forum (2013): 2
Scopus rating (2012): 2.744 1.608
Publication Forum (2012): 2
Scopus rating (2011): 2.742 1.815
Scopus rating (2010): 2.372 1.46