

## Publication list - Aatto Laaksonen - September 2022

### 2022

*Francesca Mocci, Leon Engelbrecht, Chiara Olla, Antonio Cappai, Maria Francesca Casula, Claudio Melis, Luigi Stagi, Aatto Laaksonen and Carlo Maria Carbonaro*

Carbon Nanodots from in Silico Perspective

*Chemical Reviews*, 2022, 122(16), 13709-13799.

<https://doi.org/10.1021/acs.chemrev.1c00864>

*Fernando Luis Barroso da Silva, Carolina Correa Giron and Aatto Laaksonen*

Electrostatic Features for the Receptor Binding Domain of SARS-CoV-2 Wildtype and Its Variants. Compass to the Severity of the Future Variants with the Charge-Rule

*Journal of Physical Chemistry B*, 2022, xxx, xxx-xxx. <https://doi.org/10.1021/acs.jpcb.2c04225>

*Rong An, Aatto Laaksonen, Muqiu Wu, Yudan Zhu, Faiz Ullah Shah,*

*Xiaohua Lu and Xiaoyan Ji*

AFM probing interactions and microstructures of ionic liquids at solid surfaces

*Nanoscale*, 2022 **14**, 11098. DOI: 10.1039/d2nr02812c

*Carolina Correa Giron, Aatto Laaksonen and Fernando Luis Barroso da Silva*

Differences between Omicron SARS-CoV-2 RBD and other variants in their ability to interact with cell receptors and monoclonal antibodies

*Journal of biomolecular structure and dynamics*, 2022, Ahead-of-print 1-21.

<https://doi.org/10.1080/07391102.2022.2095305>

*Yihui Dong, Mian Gong, Faiz Ullah Shah, Aatto Laaksonen, Rong An and Xiaoyan Ji*

Phosphonium-Based Ionic Liquid Significantly Enhances SERS of Cytochrome c on TiO<sub>2</sub> Nanotube Arrays

*ACS Applied Materials & Interfaces* 2022, 14(23), 27456-27465.

<https://doi.org/10.1021/acsami.2c05781>

*Carolina Correa Giron, Aatto Laaksonen and Fernando Luis Barroso da Silva*

Differences between Omicron SARS-CoV-2 RBD and other variants in their ability to interact with cell receptors and monoclonal antibodies

*BioRxiv*, Jan 31 2022, 1-69. doi: <https://doi.org/10.1101/2022.01.29.478316>

*Yihui Dong, Aatto Laaksonen, Mian Gong, Rong An and Xiaoyan Ji*

Selective Separation of Highly Similar Proteins on Ionic Liquid-Loaded Mesoporous TiO<sub>2</sub>

*Langmuir* 2022, **38**, 3202–3211 <https://doi.org/10.1021/acs.langmuir.1c03277>

*Zhibo Zhang, Tudor Vasiliu, Fangfang Li, Aatto Laaksonen, Xiangping Zhang, Francesca Mocci and Xiaoyan Ji*

Novel artificial ionic cofactors for efficient electro-enzymatic conversion of CO<sub>2</sub> to formic acid

*Journal of CO<sub>2</sub> Utilization*, 2022, **60**, 101978

<https://doi.org/10.1016/j.jcou.2022.101978>

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*Andrei Neamtu, Francesca Mocci, Aatto Laaksonen and Fernando L. Barroso da Silva*  
Towards an optimal monoclonal antibody with higher binding affinity to the receptor-binding domain of SARS-CoV-2 spike proteins from different variants  
*BioRxiv* Jan 5, 2022, 1-59. <https://doi.org/10.1101/2022.01.04.474958>  
To be published in *Colloids and Interfaces B, Biointerfaces*

*Yihui Dong, Weifeng Lin, Aatto Laaksonen and Xiaoyan Ji*  
Complementary Powerful Techniques for Investigating the Interactions of Proteins with Porous TiO<sub>2</sub> and Its Hybrid Materials: A Tutorial Review  
*Membranes* 2022, **12**, 415. <https://doi.org/10.3390/membranes12040415>

*Fangfang Li, Aatto Laaksonen, Xiangping Zhang and Xiaoyan Ji*  
Rotten Eggs Revaluated: Ionic Liquids and Deep Eutectic Solvents for Removal and Utilization of Hydrogen Sulfide  
*Industrial & Engineering Chemistry Research*, 2022, **61**, 2643–2671  
<https://doi.org/10.1021/acs.iecr.1c04142>

*Yudi Wei, Zhongyang Dai, Yihui Dong, Andrei Filippov, Xiaoyan Ji, Aatto Laaksonen, Faiz Ullah Shah, Rong An and Harald Fuchs*  
Molecular interactions of ionic liquids with SiO<sub>2</sub> surfaces determined from colloid probe atomic force microscopy  
*Physical Chemistry Chemical Physics*, 2022, **24**, 12808–12815  
DOI: 10.1039/d2cp00483f

*Yudi Wei, Yihui Dong, Xiaoyan Ji, Faiz Ullah Shah, Aatto Laaksonen, Rong An and Kristina Riehemann*  
Detailing molecular interactions of ionic liquids with charged SiO<sub>2</sub> surfaces:  
A systematic AFM study.  
*Journal of Molecular Liquids*, 2022, **350**, 118506.  
<https://doi.org/10.1016/j.molliq.2022.118506>

Fernando L. Barroso da Silva, Carolina Corrêa Giron and Aatto Laaksonen  
Electrostatic features for the Receptor binding domain of SARS-COV-2 wildtype and its variants.  
Compass to the severity of the future variants with the charge-rule.  
*bioRxiv* (2022), 1-43. <https://doi.org/10.1101/2022.06.16.496458>

*Tudor Vasiliu, Francesca Mocci, Aatto Laaksonen, Leon De Villiers Engelbrecht and Sergiy Perepelytsya*  
Caging polycations: Effect of increasing confinement on the modes of interaction of spermidine3+ with DNA double helices  
*Frontiers in Chemistry*, 2022, **10**, 836994.  
doi: 10.3389/fchem.2022.836994

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### 2021

*Leon Engelbrecht, Francesca Mocci, Yonglei Wang, Sergiy Perepelytsya, Tudor Vasiliu and Aatto Laaksonen*

Molecular Perspective on Solutions and Liquid 2 Mixtures from Modelling & Experiment  
Chapter 3 in “*Soft Matter Systems for Biomedical Applications*”

(Bulavin, Leonid, Lebovka, Nikolai (Eds.), Springer Nature Switzerland AG, 2021

DOI : 10.1007/978-3-030-80924-9

*Francesca Mocci, Aatto Laaksonen, Leon Engelbrecht, Tudor Vasiliu and Sergiy Perepelytsya*  
DNA-polyamine interactions: Insight from 2 Molecular Dynamics simulations on the sequence-specific binding of spermidine

Chapter 4 in “*Soft Matter Systems for Biomedical Applications*”

(Bulavin, Leonid, Lebovka, Nikolai (Eds.), Springer Nature Switzerland AG, 2021

DOI : 10.1007/978-3-030-80924-9

*Alexander Lyubartsev and Aatto Laaksonen*

Inverse Problems and Hierarchical Multiscale Modelling of Biological Matter

Pages 213-238, In “*New Trends in Macromolecular and Supramolecular Chemistry for Biological Applications*”, (Marc J. M. Abadie, Mariana Pinteala, Alexandru Rotaru Editors)  
Springer Nature Switzerland AG, 2021

<https://doi.org/10.1007/978-3-030-57456-7>

*Yihui Dong, Aatto Laaksonen, Qingwei Gao and Xiaoyan Ji*

Molecular mechanistic insight into ionic strength controlled interfacial behavior of a single protein on TiO<sub>2</sub> surface

*Langmuir*, 2021, 37(39) 11499-11507.

<https://doi.org/10.1021/acs.langmuir.1c01726>

*Dovile Lengvinaite, Sonata Kvedaravičiute, Stase Bielskute, Vytautas Klimavicius, Vytautas Balevicius, Francesca Mocci, Aatto Laaksonen and Kęstutis Aidas*

Structural features of the [C4mim][Cl] ionic liquid and its mixtures with water: insight from a 1H NMR experimental and QM/MD study

*Journal of Physical Chemistry B*, 2021, 125(48), 13255-13266.

*Sten Sarman and Aatto Laaksonen*

Microscopic shear flow simulations of a biaxial smectic A liquid crystal based on the soft ellipsoid string-fluid

*Phys. Chem. Chem. Phys.*, 2021, **23**, 15183

DOI: 10.1039/d1cp00957e

*Carolina Corrêa Giron, Aatto Laaksonen and Fernando Luís Barroso da Silva,*

Up State of the SARS-COV-2 Spike Homotrimer Favors an Increased Virulence for New Variants

*Frontiers in Medical Technology* 2021, **3**, 694347.

doi: 10.3389/fmedt.2021.694347

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*Simone Mulliri, Aatto Laaksonen, Pietro Spanu, Riccardo Farris, Matteo Farci, Francesco Mingoia, Giovanni N. Roviello and Francesca Mocci*

Spectroscopic and In Silico Studies on the Interaction of Substituted Pyrazolo[1,2-a]benzo[1,2,3,4]tetrazine-3-one Derivatives with c-Myc G4-DNA

*International Journal of Molecular Sciences, 2021, 22, 6028.*

<https://doi.org/10.3390/ijms22116028>

*Tudor Vasiliu, Bogdan Florin Craciun, Andrei Neamtu, Lilia Clima, Dragos Lucian Isac, Stelian S. Maier, Mariana Pinteala, Francesca Mocci and Aatto Laaksonen*

In silico study of PEI-PEG-squalene-dsDNA polyplex formation: the delicate role of the PEG length in the binding of PEI to DNA

*Biomaterials Science, 2021, 9, 6623 – 6640.*

DOI: 10.1039/d1bm00973g

*Yong-Lei Wang, Bin Li and Aatto Laaksonen*

Coarse-grained simulations of ionic liquid materials: from monomeric ionic liquids to ionic liquid crystals and polymeric ionic liquids

*Phys. Chem. Chem. Phys., 2021, 23, 19435*

DOI: 10.1039/d1cp02662c

*Zhibo Zhang, Tudor Vasiliu, Fangfang Li, Aatto Laaksonen, Francesca Mocci, Xiaoyan Ji*

Electrochemically driven efficient enzymatic conversion of CO<sub>2</sub> to formic acid with artificial cofactors

*Journal of CO<sub>2</sub> Utilization 52 (2021) 101679.*

<https://doi.org/10.1016/j.jcou.2021.101679>

*Carolina Correa Giron, Aatto Laaksonen and Fernando Luis Barroso da Silva*

The Up state of the SARS-COV-2 Spike homotrimer favors an increased virulence for new variants

*BioRxiv, doi: <https://doi.org/10.1101/2021.04.05.438465>*

*Dong, Yihui; Laaksonen, Aatto; Huo, Feng ; Gao, Qingwei; Ji, Xiaoyan*

Hydrated ionic liquids boost the trace detection capacity of proteins on TiO<sub>2</sub> support

*Langmuir, 2021, 37, 5012–5021*

<https://doi.org/10.1021/acs.langmuir.1c00525>

*Siarhei Hrom, Vladimir V. Sizov, Oleg V. Levin, Aatto Laaksonen*

Assembly of [Ni(Schiff)] films on inert surface: a multiscale computational study

*Journal of Physical Chemistry C, 2021, 125(5), 2926-2937.*

DOI:10.1021/acs.jpcc.0c09085

*Leon de Villiers Engelbrecht, Riccardo Farris, Tudor Vasiliu, Monica Demurtas, Aatto Laaksonen, Alessandra Piras, Flaminia Cesare Marincola, Silvia Porcedda and Francesca Mocci*

Theoretical and experimental study of the excess thermodynamic properties of highly non-ideal liquid mixtures of butanol isomers + DBE.

*Journal of Physical Chemistry C (2021) 125(2), 587-600.*

DOI 10.1021/acs.jpcc.0c10076.

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*Fangfang Li, Francesca Mocci, Xiangping Zhang, Xiaoyan Ji and Aatto Laaksonen*  
Ionic liquids for CO<sub>2</sub> electrochemical reduction  
*Chinese Journal of Chemical Engineering* (2021), **31** 75-93,  
<https://doi.org/10.1016/j.cjche.2020.10.029>

*Yihui Dong, Feng Huo and Aatto Laaksonen*  
Detecting Confined Fluid Behavior by SFA: Past, Present, and Future  
*Green Energy & Environment* (2021), **6(2)**, 167-168.  
<https://doi.org/10.1016/j.gee.2020.08.002>

*Qingwei Gao; Yumeng Zhang; Aatto Laaksonen; Xiaoyan Ji; Shuangliang Zhao; Yaojia Chen; Xiaohua Lu*  
Effect of dimethyl carbonate on the behavior of water confined in carbon nanotube  
*Chinese Journal of Chemical Engineering* (2021), **31**, 177-185.  
<http://dx.doi.org/10.1016/j.cjche.2020.10.041>

### **2020**

*Sten Sarman, Yonglei Wang and Aatto Laaksonen*  
Variational Principle for Nonequilibrium Steady States Tested by Molecular Dynamics  
Simulation of Model Liquid Crystal Systems  
in *Non-Equilibrium Particle Dynamics* (Ed. Albert S. Kim), IntechOpen  
DOI: [10.5772/intechopen.80977](https://doi.org/10.5772/intechopen.80977).

*Yihui Dong, Na Wu, Xiaoyan Ji, Aatto Laaksonen, Xiaohua Lu, and Suojiang Zhang*  
Excellent Trace Detection of Proteins on TiO<sub>2</sub> Nanotube Substrates through Novel Topography Optimization  
*Journal of Physical Chemistry C*, (2020) **124** (50) 27790-27800.  
<https://doi.org/10.1021/acs.jpcc.0c08793>

*Guancong Jiang, Liangcheng Cai, Shibo Wang, Aatto Laaksonen, Xin Feng, Liwen Mu, Xiaohua Lu and Jiahua Zhu*  
Critical Role of Carbonized Cellulose in the Evolution of Highly Porous Biocarbon:  
Seeing the Structural and Compositional Changes of Spent Mushroom Substrate by Deconvoluted Thermogravimetric Analysis  
*ACS Industrial & Engineering Chemistry Research* (2020), **59(52)**, 22541-22548.  
<https://dx.doi.org/10.1021/acs.iecr.0c05174>

*Yunhao Sun, Aatto Laaksonen, Aatto, Xiaohua Lu and Xiaoyan Ji*  
How to detect possible pitfalls in ePC-SAFT modelling. 2.  
Extension to binary mixtures of 96 ionic liquids with CO<sub>2</sub>, H<sub>2</sub>S, CO, O<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>, and H<sub>2</sub>  
*ACS Industrial & Engineering Chemistry Research* (2020), **59**, 49, 21579-21591  
<https://doi.org/10.1021/acs.iecr.0c04485>

*Qingwei Gao, Yumeng Zhang, Shuting Xu, Aatto Laaksonen, Yudan Zhu, Xiaoyan Ji and Xiaohua Lu*

## **Publication list - Aatto Laaksonen - September 2022**

Physicochemical properties and structure of fluid at nano-/micro-interface: Progress in simulation and experimental study,

*Green Energy & Environment* (2020) **5**(3), 274-285.

<https://doi.org/10.1016/j.gee.2020.07.013>

*Yurij A. Dmitriev, Aatto Laaksonen and Nikolas P. Benetis*

H/D isotope effect observed in the isotropic Fermi contact interaction of formyl radical:  
Experimental and theoretical analysis of the inter- and intra-molecular dynamics

*AIP Advances*, (2020), **10**, 125309. <https://doi.org/10.1063/5.0027835>

*Yihui Dong, Xiaoyan Ji, Aatto Laaksonen, Wei Cao, Hongyan He, and Xiaohua Lu*

Excellent Protein Immobilization and Stability on Heterogeneous C-TiO<sub>2</sub> Hybrid Nanostructures: A Single Protein AFM Study

*Langmuir* (2020), **36**, 9323–9332 <https://dx.doi.org/10.1021/acs.langmuir.0c01942>

*Adina Coroaba, Dragos-Lucian Isac, Cristina Al-Matarneh, Tudor Vasiliu, Sorin-Alexandru Ibanescu, Radu Zonda, Rodinel Ardeleanu, Andrei Neamtu, Daniel Timpu, Alina Nicolescu, Francesca Mocci, Stelian S. Maier, Aatto Laaksonen, Marc Jean Medard Abadie and Mariana Pinteala*

Probing the supramolecular features via p-p interaction of a di-iminopyrene-di-benzo-18-crown-6-ether compound: experimental and theoretical study

*RSC Advances* (2020), **10**, 38304-38315.

<https://doi.org/10.1039/D0RA06929A>

*Qingwei Gao, Nanhua Wu, Yao Qin, Aatto Laaksonen, Yudan Zhu, Xiaoyan, Xiaohua Lu*

Molecular insight into wetting behavior of deep eutectic solvent droplets on ionic substrates: A molecular dynamics study

*Journal of Molecular Liquids* (2020) **319** 114298 <https://doi.org/10.1016/j.molliq.2020.114298>

*Carolina Correa Girona, Aatto Laaksonen and Fernando L. Barroso da Silva*

On the interactions of the receptor-binding domain of SARS-CoV-1 and SARS-CoV-2 spike proteins with monoclonal antibodies and the receptor ACE2

*Virus Research* (2020) **285** 198021 <https://doi.org/10.1016/j.virusres.2020.198021>

*Yang, Sheng-Chun; Li, Bin; Zhu, You-Liang; Laaksonen, Aatto; Wang, Yong-Lei*

The ENUF method - Ewald summation based on non-uniform fast Fourier transform: implementation, parallelization, and application

*Journal of Computational Chemistry* (2020) **41**, 2316-2335

<https://doi.org/10.1002/jcc.26395>

*Sun, Yunhao; Zuo, Zhida; Laaksonen, Aatto; Lu, Xiaohua; Ji, Xiaoyan*

How to detect possible pitfalls in ePC-SAFT modelling: Extension to ionic liquids

*Fluid Phase Equilibria* (2020), **519**, 112641 <https://doi.org/10.1016/j.fluid.2020.112641>

*Honglin Wang, Yanrong Liu, Aatto Laaksonen, Anna Krook-Riekkola, Zhuhong Yang,*

*Xiaohua Lu, Xiaoyan Ji*

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Carbon recycling – an immense resource and key to a smart climate engineering:  
A survey of technologies, cost and impurity impact

*Renewable and Sustainable Energy Reviews*, (2020) **131**, 110010  
<https://doi.org/10.1016/j.rser.2020.110010>

*Yong-Lei Wang, Bin Li, Sten Sarman, Francesca Mocci, Zhong-Yuan Lu, Jiayin Yuan, Aatto Laaksonen, and Michael D. Fayer*

Microstructural and Dynamical Heterogeneities in Ionic Liquids  
*Chemical Reviews* (2020), **120**, 5798–5877 <https://dx.doi.org/10.1021/acs.chemrev.9b00693>

*Han-Wen Pei, Bin Li, Aatto Laaksonen and Yong-Lei Wang*

How Molecular Chiralities of Bis(mandelato)borate Anions Affect Their Binding Structures With Alkali Metal Ions and Microstructural Properties in Tetraalkylphosphonium Ionic Liquids  
*Frontiers in Chemistry*, **8**, 65 (2020) doi: 10.3389/fchem.2020.00065

*Yonglei Wang, Bin Li, Jiayin Yuan and Aatto Laaksonen*

The Effect of Phenyl Substitutions on Microstructures and Dynamics of Tetraalkylphosphonium Bis(trifluoromethylsulfonyl)imide Ionic Liquids  
*ChemPhysChem*, (2020) **21**(11), 1202-1214.  
<https://doi.org/10.3389/fchem.2020.00065>

## 2019

*D Isac, A Airinei, D Maftei, I Humelnicu, F Mocci, A Laaksonen, M Pinteala*

On the Charge-Transfer Excitations in Azobenzene Maleimide Compounds. A Theoretical Study.  
*Journal of Physical Chemistry A* **123**(26), 5525-5536, (2019)

*YongLei Wang, Sten Sarman, Mikhail Golets, Francesca Mocci, Zhong-Yuan Lu and Aatto Laaksonen*

Multi-Granular Modelling of Ionic Liquids,  
In *Ionic Liquids* (Eds. Fehrmann & Santini) ISBN 978-3-11-058363-2 de Gruyter gmbh (2019)

*Han-Wen Pei & Aatto Laaksonen*

Feature vector clustering molecular pairs in computer simulations  
*Journal of Computational Chemistry* **40**(29), 2539-2549, 2019.

*Yihui Dong, Aatto Laaksonen, Wei Cao, Xiaoyan Ji and Xiaohua Lu*

AFM study of pH dependent adhesion of single protein to TiO<sub>2</sub> surface  
*Advanced Materials Interfaces*, **6**(14) 1900411 (2019).

*Sergiy Perepelytsya, Jozef Uličný, Aatto Laaksonen and Francesca Mocci*  
Pattern preferences of DNA nucleotide motifs by polyamines putrescine<sup>2+</sup>, spermidine<sup>3+</sup>, and spermine<sup>4+</sup>

*Nucleic Acid Research*, **47**(12), 6084-6097, 2019

*Shuai Liang, Kyle Wm Hall, Aatto Laaksonen, Zhengcai Zhang and Peter G. Kusalik*

Characterizing key features in the formation of ice and gas hydrate systems.

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*Philosophical Trans. A.* **377**(2146) 20180167 (2019)

*Chunyan Ma, Aatto Laaksonen, Chang Liu, Xiaohua Lu, and Xiaoyan Ji,*  
The Peculiar Effect of Water on Ionic Liquids and Deep Eutectic Solvents,  
*Chemical Society Reviews*, **21**, 8685-8720 (2018)

*Yihui Dong, Xiaoyan Ji, Aatto Laaksonen, Wei Cao, Rong An, Linghong Lu, Xiaohua Lu*  
Determination of the extremely small amount of protein interacting with TiO<sub>2</sub> nanotubes by  
AFM-measurement,  
*Biomaterials*, **192**, 368-376 (2019)

*Sten Sarman, Yong-Lei Wang and Aatto Laaksonen,*  
Shear flow of smectic liquid crystals based on the Gay-Berne fluid and the soft sphere string-fluid  
*Physical Chemistry Chemical Physics* **21**, 292-305 (2019)

*Mathieu Fossépré, Laurence Leherte, Aatto Laaksonen, and Daniel P. Vercauteren*  
Understanding structure and dynamics of small peptides and proteins  
through the lens of network science.  
in *Biomolecular Simulations in Drug Design*, (Eds.Gervasio & Spiwok) Wiley 2019  
doi.org/10.1002/9783527806836.ch6

### 2018

*Leon Engelbrecht, Francesca Mocci, Aatto Laaksonen and Klaus R Koch*  
A <sup>195</sup>Pt NMR and MD Simulation Study of the Solvation of [PtCl<sub>6</sub>]<sup>2-</sup> in Water-Methanol and  
Water-Dimethoxyethane Binary Mixtures,  
*Inorganic Chemistry*, **57**(19), 12025-12037 (2018)

*A. V. Egorov, E. N. Brodskaya, and A. Laaksonen*  
The Effect of Single-Atomic Ions on the Melting of Microscopic Ice Particles According to  
Molecular Dynamics Data  
*Colloid Journal* (2018), **80**(5), 484-491.

*Sten Sarman, Yonglei Wang and Aatto Laaksonen*  
Variational principle for nonequilibrium steady states tested by molecular dynamics simulation of  
liquid crystal model systems  
in *Non-equilibrium Dynamics*, Intech (2018) DOI: 10.5772/intechopen.80977

*Shen, Gulou; Laaksonen, Aatto; Lu, Xiaohua; Ji, Xiaoyan*  
Developing Electrolyte Perturbed-Chain Statistical Associating Fluid Theory  
Density Functional Theory for CO<sub>2</sub> Separation by Confined Ionic Liquids,  
*Journal of Physical Chemistry C* **122**(27), 15464-15473, (2018)

*YL Wang, YL Zhu, ZY Lu, and A. Laaksonen*  
Electrostatic Interactions in Soft Particle Systems: Mesoscale Simulations of Ionic Liquids  
*Soft Matter*, (2018), **14**(21), 4252-4267.

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*Sten Sarman, Yong-Lei Wang, Patrick Rohlmann, Sergei Glavatskikh, and Aatto Laaksonen*  
Rheology of phosphonium ionic liquids: An MD and experimental study.  
*Physical Chemistry Chemical Physics*, (2018), **20**, 10193.

### **2017**

*Yonglei Wang, Aatto Laaksonen and Michael D. Fayer*  
Hydrogen Bonding vs  $\pi$ - $\pi$  Stacking Interactions in Imidazolium-Oxalatoborate Ionic Liquid  
*Journal of Physical Chemistry B* (2017), **121**(29), 7173-7179

*Sten Sarman and Aatto Laaksonen,*  
Director Orientation Relative to External Dissipative Fields in Nematic & Cholesteric Liquid Crystals  
*Computational Methods in Science and Technology*, **23**, 239 (2017)

*M. Rebic, F. Mocci, J. Ulicny, A. Lyubartsev, A. Laaksonen,*  
Coarse-Grained Simulation of Rodlike Higher-Order Quadruplex Structures at Different Salt Concentrations.  
*ACS Omega* (2017), **2**(2), 386-396.

*Wang, Yong-Lei; Golets, Mikhail; Li, Bin; Sarman, Sten; Laaksonen, Aatto*  
Interfacial Structures of Trihexyltetradecylphosphonium-bis(mandelato)borate Ionic Liquid Confined between Gold Electrodes  
*ACS Applied Materials & Interfaces* (2017), **9**(5), 4976-4987.

*Driver, G. W.; Huang, Y.; Laaksonen, A.; Sparrman, T.; Wang, Y.-L.; Westlund, P.-O.*  
Correlated/non-correlated ion dynamics of charge-neutral ion couples:  
the origin of ionicity in ionic liquids  
*Physical Chemistry Chemical Physics* (2017), **19**(7), 4975-4988.

### **2016**

*Atzori, Alessio; Liggi, Sonia; Laaksonen, Aatto; Porcu, Massimiliano; Lyubartsev, Alexander P.; Saba, Giuseppe; Mocci, Francesca*  
Base sequence specificity of counterion binding to DNA: what can MD simulations tell us?  
*Canadian Journal of Chemistry* (2016), **94**(12), 1181-1188.

*Wang, Yong-Lei; Sarman, Sten; Kloo, Lars; Antzutkin, Oleg N.; Glavatskikh, Sergei; Laaksonen, Aatto*  
Solvation structures of water in trihexyltetradecylphosphonium-orthoborate ionic liquids  
*Journal of Chemical Physics* (2016), **145**(6), 064507/1-064507/11.

*Golets, M.; Shimpi, M. R.; Wang, Y.-L.; Antzutkin, O. N.; Glavatskikh, S.; Laaksonen, A.*  
Understanding the thermal decomposition mechanism of a halogen-free chelated orthoborate-based ionic liquid: a combined computational and experimental study  
*Physical Chemistry Chemical Physics* (2016), **18**(32), 22458-22466.

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*Matúš Rebič, Aatto Laaksonen, Jiří Šponer, Jozef Uličný and Francesca Mocci*  
Molecular Dynamics Simulation Study of Parallel Telomeric DNA Quadruplex at Different Ionic Strengths. Evaluation of Water and Ion Models  
*Journal of Physical Chemistry B* (2016), 120(30), 7380-7391.

*Vereshchagin, Anatoliy A.; Sizov, Vladimir V.; Verjuzhskij, Mikhail S.; Hrom, Siarhei I.; Volkov, Alexey I.; Danilova, Julia S.; Novozhilova, Maria V.; Laaksonen, Aatto; Levin, Oleg V*  
Interaction of amines with electrodes modified by polymeric complexes of Ni with salen-type ligands  
*Electrochimica Acta* (2016), 211, 726-734.

*Sten Sarman and Aatto Laaksonen*  
Thermomechanical coupling in coarse grained cholesteric liquid crystal model systems with pitches of realistic length  
*Physical Chemistry Chemical Physics* (2016), 18(25), 16822-16829.

*Yong-Lei Wang, Manishkumar R. Shimpi, Sten Sarman, Oleg N. Antzutkin, Sergei Glavatskikh, Lars Kloo and Aatto Laaksonen.*  
Atomistic Insight into Tetraalkylphosphonium-Bis(oxalato)borate Ionic Liquid/Water Mixtures II. Volumetric and Transport Properties.  
*Journal of Physical Chemistry B*, (2016), 120(30), 7446-7455

*Fossépré, Mathieu; Leherte, Laurence; Laaksonen, Aatto; Vercauteren, Daniel*  
Multiscale design of coarse-grained elastic network-based models for the  $\mu$  opioid receptor flexibility  
*Journal of Molecular Modeling* - (2016), 22(9), 1-20

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