ZdeněkPreisler

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Physicist. I am an expert in statistical mechanics/physics and computer simulations. I make predictive mathematical models of complex systems. Most recently I apply machine learning/deep learning in my research.

Technical Expertise

Over 10 years of experience developing codes for scientific applications

• **data analysis** • **advanced algorithms** • **scientific computing** • **linux administrator** • **HPC environment**

• Experience with a wide range of simulation techniques: **Monte Carlo**, **Molecular dynamics**, Brownian dynamics, kinetic Monte Carlo • both **equilibrium** and **out-of-equilibrium** statistical mechanics • Expert in calculation of entropies and free energies • machine learning/deep learning implemented using **TensorFlow**.

Programming

I develop optimized, computationally intensive codes in **C** [10+ years]

• **Python** [10+years] • **parallel programming [OpenMP, MPI, OpenCL]** • **graphics [OpenGL, postscript, Povray]**

scripting, bash, zsh, LaTeX, low level programming, Assembly, SIMD instructions, Arduino, git, Mathematica, scipy, matplotlib, scikit, NumPy, SciPy, pandas, Jupyter Notebook

Skills

I am used to work independently as well as in teams of people with various backgrounds

• **critical & analytical thinking** • **writing and oral communication skills** • **theoretical support and guidance**
• **publication quality graphs and graphics** • **training and supervision of students and users**

4 Languages

English [Fluent], **Czech** [Native], **Italian** [Fluent], **French** [Conversational]

Work Experience

Lawrence Berkeley National Lab, Berkeley, CA, USA

i) **Postdoctoral Research Fellow**, Molecular Foundry — Nov 2016 - current

- Work in an interdisciplinary DOE user facility in the group of *Stephen Whitelam*
- Applying machine learning to recognition and generation of solid phases (CNN, GAN, VAE), and automating of phase diagram calculations
- Part of a multidisciplinary team providing new capabilities to the Molecular Foundry: A combinatorial approach to multifunctional porous graphitic materials; I am providing a theoretical framework for the project
- Theoretical predictions for self-assembly of DNA nanoparticles
- Developing trajectory sampling schemes using large deviation principle for stochastic systems

Utrecht University, The Netherlands

ii) **Postdoctoral Research Fellow**, Debye Institute for Nanomaterial Science — Dec 2013 - Dec 2015

- Collaboration with experimentalists on self-propelled rods; *prof. Marjolein Dijkstra*
- Calculating Lyapunov exponents for deterministic chaotic systems under shear
- Statistical mechanical descriptions of active matter
- Funded by Dutch Foundation for Fundamental Research of Matter (FOM) to study self-assembly

Education

Università di Roma "Sapienza", Italy

Doctor of Philosophy, Physics — Nov 2010 - Feb 2014

- Marie Curie Initial Training Network COMPLOIDS - Prestigious European training program for early stage researchers; Collaboration with number of universities and industries across Europe
- Predicting phase behavior of One Patch colloidal particles, *prof. Francesco Sciortino*

M.Sc., Physical Chemistry, Charles University in Prague, Czech Rep. — Sep 2008 - Dec 2010

- Computer simulation of branched polymers on lattice; *K. Procházka*

ERASMUS, Université de Bordeaux I, France — Sep 2008 - June 2009

- Research project improving existing water model; *P. Bopp*

B.Sc., Chemistry in Natural Sciences, Charles University in Prague, Czech Rep. — Sep 2005 - June 2008

Rotary Youth Exchange, Keen High school, Keen, NH — Sep 2003 - June 2004

Interests & Research Interests

AI, machine learning/deep learning, dynamical systems, large deviation theory, equilibrium/out-of-equilibrium statistical mechanics, thermodynamics, methodology, self-assembly, phase behavior, crystallization, ergodicity, active matter, glasses

Publications

[1] Z. Preisler, B. Sacca, S. Whitelam
Irregular model DNA particles self-assemble into a regular structure
Soft Matter, **2017**,13, 8894-8902

[2] Z. Preisler, T. Vissers, F. Smallenburg and F. Sciortino
Crystals of Janus colloids at various interaction ranges
J. Chem. Phys., **2016,** *145,* 064513

[3] H. R. Vutukuri, Z. Preisler, T. H. Besseling, A. van Blaaderen, M. Dijkstra, W. T. S. Huck
Dynamic self-organization via collective motion of self-propelled colloidal rods
Soft Matter, **2016,** *12,* 9657-9665

[4] Z. Preisler, M. Dijkstra
Configurational entropy and effective temperature in systems of active Brownian particles
Soft Matter, **2016,** *12,* 6043-6048

[5] Z. Preisler, T. Vissers, G. Munaò, F. Smallenburg and F. Sciortino
Equilibrium phases of one-patch colloids with short-range attractions
Soft Matter, **2014**,*10*, 5121-5128

[6] T. Vissers, F. Smallenburg, G. Munaò, Z. Preisler, and F. Sciortino
Cooperative polymerization of one-patch colloids
J. Chem. Phys., **2014**, *140* 144902

[7] Z. Preisler, T. Vissers, F. Smallenburg, G. Munaò and F. Sciortino
Phase diagram of one-patch colloids forming tubes and lamellae
J. Phys. Chem. B, **2013**, *117*, 9540-9547

[8] T. Vissers, Z. Preisler, F. Smallenburg, M. Dijkstra and F. Sciortino
Predicting crystals of Janus colloids
J. Chem. Phys., **2013**, *138*, 164505

[9] G. Munaò, Z. Preisler, T. Vissers, F. Smallenburg and F. Sciortino
Cluster formation in one-patch colloids: low coverage results
Soft Matter, **2013**, *9*, 2652-2661

[10] Z. Preisler, P. Košovan, J. Kuldová, F. Uhlík, Z. Limpouchová, K. Procházka and F. A. M. Leermakers
Depletion profiles for dilute solutions of linear chains, stars and H-branched molecules by self-consistent field calculations and Monte Carlo simulations
Soft Matter, **2011,** *7,* 10258-10265

Selected Conferences & Workshops

SIAM, Society for Industrial and Applied Mathematics, Portland, July 2018

Liquid Matter Conference, Lisbon, July 2014

International Soft Matter Conference, Rome, September 2013

Physics of Complex Colloids, Ljubljana, May 2013

Liquid Matter Conference, Vienna, 2011

Emergent Colloidal Dynamics Far From Equilibrium, Lausanne, Switzerland, April 2014

Physics of Complex Colloids, Varenna, Italy, July 2012

International Workshop on Dynamics in Viscous Liquids, Rome, March 2011

Novel Simulation Approaches to Soft Matter Systems, Dresden, September 2010

POLYAMPHI Summer School 2007, Biezenmortel, Netherlands, October 2007