

GRK 2516 Soft Matter Seminar

Nov. 30, 2023 at 2:30 p.m.
Minkowski Room, 05-119, Staudingerweg 7

Research seminar of the DFG Research Training Group GRK 2516 (<https://grk2516.uni-mainz.de>).

Dijkstra, Marjolein
Computational Condensed Matter, Utrecht
University

Accelerating the design of soft materials using machine learning

Predicting the emergent properties of a material from a microscopic description is a scientific challenge. Machine learning and reverse-engineering have opened new paradigms in the understanding and design of materials. However, this approach for the design of soft materials is highly non-trivial. The main difficulty stems from the importance of entropy, the ubiquity of multi-scale and many-body interactions, and the prevalence of non-equilibrium and active matter systems. The abundance of exotic soft-matter phases with (partial) orientation and positional order like liquid crystals, quasicrystals, plastic crystals, along with the omnipresent thermal noise, makes the classification of these states of matter using ML tools highly non-trivial. In this talk, I will address questions like: Can we use machine learning to autonomously identify local structures [1,2], detect phase transitions [1], classify phases and find the corresponding order parameters [2], can we identify the kinetic pathways for phase transformations [1], and can we use machine learning to coarse-grain our models [3,4,5]? Finally, I will show in this lecture how one can use machine learning to reverse-engineer the particle interactions to stabilize nature's impossible phase of matter, namely quasicrystals [6]?

[1] An artificial neural network reveals the nucleation mechanism of a binary colloidal AB13 crystal

G.M. Coli and M. Dijkstra, *ASC Nano* 15, 4335-4346 (2021).

[2] Classifying crystals of rounded tetrahedra and determining their order parameters using dimensionality reduction

R. van Damme, G.M. Coli, R. van Roij, and M. Dijkstra, *ACS Nano* 14, 15144-15153 (2020).

[3] Machine learning many-body potentials for colloidal systems

G. Campos-Villalobos, E. Boattini, L. Filion and M. Dijkstra, The Journal of Chemical Physics 155 (17), 174902 (2021).

[4] Machine-learning effective many-body potentials for anisotropic particles using orientation-dependent symmetry functions

G. Campos-Villalobos, G. Giunta, S. Marín-Aguilar and M. Dijkstra, The Journal of Chemical Physics 157 (2), 024902 (2022).

[5] Coarse-Grained Many-Body Potentials of Ligand-Stabilized Nanoparticles from Machine-Learned Mean Forces

G. Giunta, G. Campos-Villalobos, and M. Dijkstra, ACS Nano (2023).

[6] Inverse design of soft materials via a deep learning-based evolutionary strategy

G.M. Coli, E. Boattini, L. Filion, and M. Dijkstra, Science Advances 8 (3), eabj6731 (2022).