

Machine learning and Inverse design of soft materials

Monday, 11 April 2022 17:00 (1 hour)

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, the soft-matter field has lagged far behind in embracing this approach for materials design. 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], detect phase transitions, classify phases and find the corresponding order parameters [2] in soft-matter systems, can we identify the kinetic pathways for phase transformations [3], and can we use machine learning to coarse-grain our models? [4,5] Finally, I will show how one can use machine learning to reverse-engineer the particle interactions to stabilize nature's impossible phase of matter, namely quasicrystals? [6]

[1] Unsupervised learning for local structure detection in colloidal systems

E. Boattini, M. Dijkstra, and L. Filion *The Journal of Chemical Physics* 151, 154901 (2019).

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

G.M.Coli and M. Dijkstra, *ASC Nano* 15 (3), 4335-4346 (2021).

[4] 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).

[5] Machine learning free-energy functionals using density profiles from simulations

P. Cats, S. Kuipers, S. de Wind, R. van Damme, G.M. Coli, M. Dijkstra and R. van Roij, *APL Materials* 9, 031109 (2021).

[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).

Poster title

Primary author: DIJKSTRA, Marjolein (Utrecht University)

Presenter: DIJKSTRA, Marjolein (Utrecht University)

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