FLAIR

Colloquium

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Investigating long-range interactions in molecules and materials with machine learning potentials

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The steady growth of machine learning methods for atomistic modelling has opened many new opportunities for research in materials science, especially for applications requiring large cell sizes, long timescales, and first-principles accuracy. However, while modern ML-PES methods have gotten more and more accurate, reliable, user-friendly, and easy to apply to new systems, this is usually only true when using them to model short-range interactions. In the (many) systems where long-range interactions such as electrostatics, induction, and dispersion are important or even decisive in determining the system behaviour, we have to rely on often manual, hand-tuned and system-dependent approaches. In this talk, I will present a few examples of such approaches I have applied in my research in modelling both molecular systems and materials, while highlighting the common themes that unite these (traditionally separate) research areas in the context of atomistic simulation. In addition, I will show how these approaches can help us gain a better insight into a material's behaviour by computing properties not accessible from the PES alone.

Max Veit obtained his bachelor's degree in physics and in computer science from the University of Minnesota, Twin Cities in 2014, and continued to a master's and finally a PhD at the University of Cambridge in 2018. His PhD work with Gábor Csányi focused on developing machine learning (ML) models for accurate atomistic simulation of molecular liquids. Before joining Miguel Caro's group at Aalto University in 2022, he was a postdoc in the COSMO group at EPFL, led by Michele Ceriotti, where he worked on improving the efficiency and expanding the capability of atomistic ML simulations for both molecular and condensed-phase systems. Now, in Miguel Caro's group, he is working to apply such physics-inspired ML models to practical problems that push the frontiers of chemical complexity, system size, and predictive capability currently achievable with ML atomistic simulations.

Interessierte sind herzlich eingeladen !

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