Joint Theory Seminar
European XFEL, CFEL & University of Hamburg

Thursday, 16 February 2023, 16:00

CFEL (Building 99), Room IV (1st floor), DESY

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"Physics-Informed Neural Network Models for Predicting the Electronic Structure of Matter"

In this talk, I will present our recent advancements in utilizing Artificial Intelligence (AI) to significantly enhance the efficiency of electronic structure calculations [1]. In particular, I will focus on our efforts to accelerate Kohn-Sham density functional theory calculations at finite temperatures by incorporating deep neural networks within the Materials Learning Algorithms framework [2,3].
Our results demonstrate substantial gains in calculation speed for metals across their melting point. Furthermore, our implementation of automated machine learning has resulted in significant savings in computational resources when identifying optimal neural network architectures, thereby laying the foundation for large-scale AI-driven investigations [4]. I will also showcase our most recent breakthrough, which enables neural-network-driven electronic structure calculations for systems containing over 100,000 atoms [5]. Finally, I will provide an outlook on the potential of physics-informed neural networks for solving time-dependent Kohn-Sham equations, which describe electron dynamics in response to incident electromagnetic waves [6].

[1] L. Fiedler, K. Shah, M. Bussmann, A. Cangi, Phys. Rev. Materials 6, 040301, (2022).
[2] A. Cangi, J. A. Ellis, L. Fiedler, D. Kotik, N. A. Modine, V. Oles, G. A. Popoola, S. Rajamanickam, S. Schmerler, J. A. Stephens, A. P. Thompson, MALA, https://doi.org/10.5281/zenodo.5557254 (2021).
[3] J. A. Ellis, L. Fiedler, G. A. Popoola, N. A. Modine, J. A. Stephens, A. P. Thompson, A. Cangi, Phys. Rev. B 104, 035120 (2021).
[4] L. Fiedler, N. Hoffmann, P. Mohammed, G. A. Popoola, T. Yovell, V. Oles, J. A. Ellis, S. Rajamanickam, A. Cangi, Mach. Learn.: Sci. Technol. 3 045008 (2022).
[5] L. Fiedler, N. A. Modine, S. Schmerler, D. J. Vogel, G. A. Popoola, A. P. Thompson, S. Rajamanickam, A. Cangi, arXiv:2210.11343 (2022).
[6] K. Shah, P. Stiller, N. Hoffmann, A. Cangi, Physics-Informed Neural Networks as Solvers for the Time-Dependent Schrödinger Equation, NeurIPS Machine Learning and the Physical Sciences, arXiv:2210.12522 (2022).

Hosts: Beata Ziaja-Motyka and Nils Brouwer

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