Computational Materials Science Seminar

Thursday, December 5, 4 p.m.

Offline and Online Room B2-3005

Molecular dynamics modeling of carbon-based materials: current trends and challenges

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Speaker introduction

Graduated from Moscow Institute of Physics and Technology in 2014, received PhD at the same University in 2018.
Currently deputy head of Computational materials design laboratory (MIPT).

Research interests:
› Computational materials science using classical molecular dynamics and density functional theory.
› Phase transitions, especially in carbon and carbonaceous systems.
› Supramolecular assemblies in aqueous solutions, classical nucleation theory.

Seminar abstract

Classical molecular dynamics (MD) is one of the few computational approaches capable of modeling carbon materials on a nanosecond timescale with atomistic precision. Significant efforts have been devoted to developing universal interatomic potentials for carbon. However, this task has historically been highly challenging due to the vast number of carbon allotropes and the complexity of its phase space. A continuously growing variety of available reactive interatomic potentials for carbon required careful validation [1,2] for a particular molecular system and pressure-temperature conditions. Fortunately, recent advances in machine-learning-based interatomic potentials are beginning to address these challenges, offering promising improvements [3].
In this talk, we will explore the history of carbon interatomic potential development and discuss the future of classical MD in the context of machine learning-driven approaches.

References

[1] C Tomas et al "Graphitization of amorphous carbons: A comparative study
of interatomic potentials" Carbon, 109, 681 (2016)
[2] N Orekhov et al, "High temperature pure carbon nanoparticle formation: Validation of AIREBO and ReaxFF reactive molecular dynamics", Carbon 170, 606 (2020)
[3] Batatia, Ilyes, et al. "A foundation model for atomistic materials chemistry." arXiv preprint arXiv:2401.00096 (2023)

Seminar

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