Universität Bielefeld Fakultät für Physik

Condensed Matter Theory

Seminar

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The Molecular Dynamics Method: Past, Present and Future Examples from Carbon Materials Science

Molecular Dynamics (MD) is a powerful and instructive tool in materials science, revealing the atomistic mechanism by which solids, liquids and gases evolve as a function of time. By controlling quantities such as pressure, temperature, density and chemical potential, the microscopic origin of macroscopic behaviour can be studied and interpreted. This presentation will provide a perspective on six decades of progress in MD, using the prism of pure carbon materials as an exemplar system. It will chart the methods that have been developed, and will highlight the importance of benchmarking and machine learning for future progress. Cases studies from nanoporous carbons and diamond-like tetrahedral amorphous carbon will be presented as specific examples of the predictive power of MD, linking conceptual models with experimental results.

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