Seminar in Physical Chemistry

Ben-Gurion University of the Negev
Department of Chemistry

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Time 16:00

Bldg. **29** Room **307**

Unraveling microscopic origins of complex behavior in sodium

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Understanding microscopic origins of complex physicochemical processes in elements is the key for designing new technologically important materials. Currently the application of computer simulations for modeling behavior of materials is limited because of the inadequacy of empirical potentials to describe interatomic interactions and the computational expense of ab-initio simulations. Neural-network representation of potential energy surfaces is an emerging methodology that combines the accuracy of first-principle methods with the high computational efficiency of empirical potentials. It enabled us to perform molecular dynamics simulations of high-pressure high-temperature processes in sodium on previously inaccessible time and length scales.

In this talk, I will discuss new insights into the electronic-structure origin of the anomalous melting behavior of dense sodium.