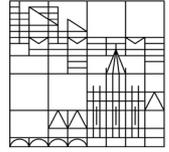


Physikalisches Kolloquium

Universität
Konstanz



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From Levinthal's paradox to the enigma of missing structures: Using Minima Hopping to gain insight into potential energy landscapes

The potential energy surface of molecules and solids is a complex high-dimensional function with a huge number of minima. The global minimum represents the ground state and all other minima meta-stable structures. I will first discuss whether and how these minima can be found in computer simulations. The next question is then whether nature can always find theoretically discovered structures. I will present a system, namely the $\text{Si}_{20}\text{H}_{20}$ dodecahedron, which can not find its ground state on a realistic experimental time scale. I will also present solids which are frozen into meta-stable structures and can not relax into their zero temperature ground state on an experimental time scale. Finally, I will discuss methods to find transformation pathways between different structures.

Host:

Prof. Zilberberg

Organisator:

Prof. Bechinger

Di 09.04.2024

15:15 Uhr

P 603

im Anschluss Getränke und Snacks