Physikalisches Kolloquium

Di, 17.05.22 15:15 Uhr R513 Kaffee/Tee im Anschluss

Hard sphere crystal-fluid interfaces





Prof. Dr. Martin Oettel

Computational Soft Matter and Nano-Science Universität Tübingen

Universität Konstanz

The classical condensed phases of matter: Hard spheres and other simple model systems

In standard lectures on condensed matter physics for undergraduate students, solids at finite temperatures are introduced through a simple harmonic picture: atoms are trapped in an energetic minimum which mainly arises owing to the potential energy with their neighbors, and they perform small vibrations eventually leading to the picture of a free phonon gas. The liquid state is usually neglected altogether.

Here I show that our current understanding of correlations in liquids and solids has come through the study of hard spheres (billiard balls) and that entropy is a major factor in understanding these. A successful analytic theory is classical density functional theory which for hard spheres is built on mainly geometric insights. For the crystal phase, it leads to surprising insights on the role of simple defects (vacancies). Furthermore, I discuss a novel strategy to improve classical density functional theory for other systems using methods of machine learning.