

Theoriekolloquium

Am **17. November 2022** um **14.15 Uhr** im **Raum W2 1-143** hält

Herr Jun.-Prof. Dr. Tim Neudecker (Uni Bremen)

einen Vortrag mit dem Titel

The Pressure Is On - Simulating Molecules and Materials in the Gigapascal Regime

The diamond anvil cell is an experimental tool that allows to subject materials to pressures as high as in Earth's core. Under such extreme conditions, the structural, electronic and spectroscopic properties of materials change dramatically and chemical reactions that are otherwise impossible can be initiated. Our group has developed computational techniques for the simulation of high-pressure chemistry, which can be used to gain a fundamental understanding of the molecular processes occurring in the gigapascal regime. In this talk, the theoretical foundations of these approaches are introduced and recent applications in computational high-pressure chemistry and materials science, ranging from molecular pressure sensors to structural properties of crystals under pressure, are pointed out.

Interessierte sind herzlich eingeladen.

gez. Prof. Dr. Caterina Cocchi