

NUSTAR Seminar

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Wednesday, January 30, 2019 at 14:30 p.m.

Seminar room „Theory“, SB3 3.170a
Planckstraße 1, 64291 Darmstadt

„Predicting Properties of Elusive Elements with Accurate ab-initio Methods“

Many heavy and superheavy elements are inaccessible for precise experimental measurements of their physical and chemical properties. For example, we have no reliable melting temperature for the radioactive rare gas radon - the only available experiment is over 100 years old - and also the heaviest member of the periodic table, oganesson, is still out of reach for experimental investigation.

However, with state-of-the-art quantum chemical methods it is possible to compute the electronic structure of atoms with high accuracy, incorporating spin-orbit relativistic effects which are crucial for the heaviest elements.

This talk describes an methodology for melting simulations of noble-gas solids based on ab-initio interatomic potentials, the bulk properties and the atomic electronic structure of the heavier rare gases.

While discussing the outcomes, a century-old experiment will be put to test and the outstanding properties the element oganesson will be highlighted.