CFEL SCIENCE

SEMINAR

2 December 2021, 10:00–11:00h

Zoom virtual meeting https://desy.zoom.us/j/83631120632

(Meeting ID: 836 3112 0632 Password: 235618)

Jan Hermann

Freie Universität Berlin

Pushing the accuracy–efficiency boundary of electronic-structure calculations

I will talk about two new methods for electronic-structure calculations. The first is a deep-learning approach to quantum Monte Carlo, which provides highly accurate ground-state electronic wave functions and energies, and offers an alternative to the large and inefficient expansions in Slater determinants used in high-accuracy quantum chemistry. The second is a semi-empirical density-functional model of van der Waals interactions in molecules and materials that unifies many-body atomic approaches and nonlocal density functionals to offer a general, efficient, and accurate method.

Host: Jochen Küpper/ CFEL Molecular and Ultrafast Science Seminar