

Einladung zum
ICP-Kolloquium (ICP Seminarraum + Hybrid via Zoom)

Prof. Dr. Andreas Köhn
Universität Stuttgart
Institut für Theoretische Chemie

hält am

Montag, 19.12.2022, 14:00 Uhr
ICP Seminarraum 1.079, Allmandring 3

und via zoom

<https://us06web.zoom.us/j/83814909766?pwd=b1RrdnZnLytJQlhcCN3hUSCtPSXN6QT09>

Meeting-ID 838 1490 9766

Kenncode 436227

einen Vortrag über das Thema:

“Coupled-cluster theory (for molecules and prospects for its application in the condensed phase)”

Abstract:

Coupled-cluster theory is the approach of choice for solving the electronic Schrödinger equation of molecular systems with high accuracy. I will give an outline of the basic theory and will address three main challenges: (a) reaching the complete basis set limit, (b) treatment of open-shell systems, and (c) reduction of the computational scaling behavior. In particular, the latter is of interest when considering the prospects of applying coupled-cluster theory to problems in the condensed phase.

Interessenten sind herzlich eingeladen.

Prof. Dr. C. Holm
Dr. Rudolf Weeber
Dr. Alexander Schlaich