UNIVERSITÄT DUISBURG ESSEN

Offen im Denken

Theorie-Kolloquium SS 2021

Fr 02.07.2021, **14:30-15:45**

Online (URL in E-Mail)

udue.de/TheoKoll

Beginn: 14:30 Uhr

Recent Progress in Auxiliary-Field Quantum Monte Carlo

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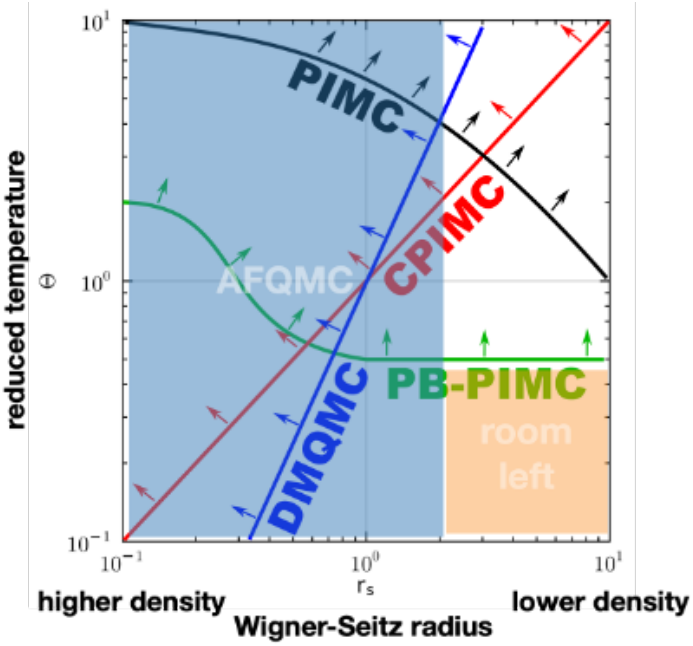

The development of quantum chemistry tools has been focused mainly on the electronic ground state within the Born-Oppenheimer approximation. Over the past few years, several research groups have extended the ground state electronic quantum chemistry methods to finite temperature as well as coupled electron-phonon systems. In this talk, we will discuss how these generalizations are achieved within the framework of auxiliary-field quantum Monte Carlo (AFQMC). We will first discuss the performance of AFQMC for the uniform electron gas in the warm-dense regime. We verify the known exchange-correlation parametrization in the regimes where no other QMC methods can run. Then, we discuss how one can seamlessly combine the electronic AFQMC approach with bosonic sampling for coupled electron-phonon problems. We test our algorithm on the Hubbard-Holstein model with various electron-phonon coupling strengths, demonstrating regimes that AFQMC can struggle as well as regimes that it can work well. Lastly, if there is enough time, we will discuss a potentially interesting connection between AFQMC and quantum computing.