Many of the most important challenges our society has to face in the next decades are related to materials science. Computer simulations are expected to contribute significantly to the development and understanding of materials that exhibit specific properties to fulfil key tasks in more efficient and novel devices as well as chemical processes. The properties of most materials arise largely from the quantum mechanics of their constituent electrons under the influence of the electric field of the nuclei. Consequently, the accurate solution of the underlying many-electron Schrödinger equation is at the heart of ab initio calculations in materials science.

A promising class of approximations widely used in quantum chemistry to solve the many-electron Schrödinger equation is the so-called coupled-cluster family of methods. These methods achieve for a large class of systems a high accuracy at a comparably moderate cost. Here, we report results of state-of-the-art simulations employing high performance computing resources to produce reliable benchmark results of molecules and surfaces containing more than 50 atoms. These benchmark results are needed to advance computationally more efficient but less accurate theories that can be improved by adjusting parameters and will ultimately be needed to model real materials in their full complexity.

The presentation will introduce the employed massively parallel tensor framework CTF. This library is used for the tensor contractions in our computer implemenation of coupled cluster theory for periodic systems using a plane wave basis ser. CTF is highly scalable and allows efficient tensor contractions on thousands of cores.