Quantum Monte Carlo Modeling for Nanotechnologies

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Explicitly correlated many-body Quantum Monte Carlo (QMC) techniques as a tool for ultra-accurate modeling of electronic structure of systems of relevance in nanotechnology will be highlighted. Applications of QMC methods to organometallic cluster systems with transition metal atoms will be used to demonstrate the accuracy and computational feasibility. It will be shown, that these techniques not only surpass in accuracy the customarily used mean field methods, such as the widely used density functional method (DFT), by about an order of magnitude but, in addition, they provide results which may differ from the simpler mean field methods even qualitatively. Consequences for applications in spintronics applications will briefly be mentioned. With virtues of QMC methods such as asymptotic scaling with system size similar to mean field methods, communications overhead smaller than in mean field methods and steady increase of available computer power, these methods hold the promise to eventually replace the traditional electronic structure methods, such as the DFT methods, in the next decade. Finally, the outlook of using QMC methods for extremely large systems on different types of platform ranging from supercomputers, grids, to cloud-computing will be discussed.