

Theorieseminar Pradipta Samanta

Title:

Response formalism within full configuration interaction quantum Monte Carlo: Calculation of static polarizability

Abstract:

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Full Configuration Interaction Quantum Monte Carlo method (FCIQMC) is a projector quantum Monte Carlo approach constructed in a discrete basis of antisymmetric, orthogonal Slater determinants. FCIQMC has been successfully applied to calculate highly accurate ground and excited state energies of molecules, and expectation values of first order properties such as dipole moment. In this talk the newly developed response formalism within the FCIQMC framework will be presented. This formalism is used to calculate linear response such as static dipole polarizability for diatomic molecules. The accuracy of FCIQMC is thus tested in predicting response properties in comparison to other methods in quantum chemistry.