On behalf of the

Science College CMS
Vienna Computational Materials Laboratory
and Center for Computational Materials Science

we cordially invite you to the following seminar

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Wave function based treatment of electronic correlation in solids

The use of wave function based methods to treat electronic correlation, such as Møller-Plesset perturbation theory and coupled-cluster theory, is common practice in the field of computational quantum chemistry. Due to the computational cost involved, however, these methods have rarely been applied to extended systems.

We have implemented the second-order Møller-Plesset perturbation theory (MP2) and an approximation to the coupled-cluster doubles (CCD) theory including only ring diagrams in the amplitude equations within the framework of the full-potential Projector-Augmented-Wave (PAW) method, using periodic boundary conditions and a plane wave basis set. The latter method goes beyond the socalled direct-random-phase approximation (RPA) by incorporating an exchangelike term that originates from the CCD energy expression. We call the exchangelike term second-order screened exchange (SOSEX), since the corresponding diagram is reminiscent of the exchange-like Goldstone diagram in second-order perturbation theory, albeit with one Coulomb line replaced by a screened Coulomb interaction.

We show that MP2 and RPA+SOSEX allow for an accurate description of electronic correlation in atoms and solids at least in those cases where the groundstate is well approximated by a single reference determinant.

Date: Monday, Dec 13, 2010 16:00

Location: Seminar room 138C (TU Freihaus 9. Stock, gelb)
A-1040 Wien, Wiedner Hauptstaße 8-10