VIENNA COMPUTATIONAL MATERIALS LABORATORY

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Applying the RPA to Complex Systems in Materials Science

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Computational Materials Physics

DATE / TIME	26.03.2012, 04:00 p.m. (CET)
LOCATION	Josef-Stefan-Hörsaal, vormals kleiner Hörsaal der Materialphysik, 3. Stock, Boltzmanngasse 5/Strudelhofgasse 4
ABSTRACT	For ab initio electronic structure calculations, the random phase approximation (RPA) to the correlation energy is a suitable complement to the exact exchange energy. Lattice constants, atomization energies of solids and heats of formations are evaluated using this approximation and show very good agreement with experiment. Since the method is fairly efficient and handles ionic, metallic, and van der Waals bonded systems equally well, it is a very promising choice to improve upon density functional theory calculations, without resorting to more demanding diffusion Monte Carlo (DMC) or quantum chemical methods. In light of these findings we investigate carbon-water interaction for the case of water adsorption on a graphene sheet. We compare our results to results obtained with DMC. As a second application of RPA to complex systems we discuss the adsorption of a carbon-monoxide (CO) molecule on Cu, late 4d metals and Pt surfaces.