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

Dr. Georg Madsen

ICAMS, Univ. Bochum, Germany

MGGAs for gold clusters and dispersive interactions

Recent developments in local functionals including the kinetic energy density, so-called meta-generalized gradient approximations (MGGAs), are described. It is shown how MGGAs can solve the long-standing problem of the cross over between 2D and 3D structure for cationic and anionic gold clusters. The MGGAs stronger tendency towards 3D structures lies in their smaller gradient enhancement, but contrary to GGAs with smaller gradient enhancements, MGGAs do not overestimate the atomization energy.
Furthermore, we find that closed shell interactions are fingerprinted in the kinetic energy density and that MGGAs have enough flexibility to treat correctly both the covalent and the short range part of the dispersive interactions in layered solids such as Graphite, h-BN and MoS_2.

Ferrighi, Hammer, Madsen, J. Am. Chem. Soc. **2009**, *131*, 10605 Madsen Ferrighi, Hammer, J. Phys. Chem. Lett. **2010**, *1*, 515

Date: Monday, Oct 11, 2010 16:00

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