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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First-Principles Modeling of Metal-Molecule Interfaces: Energy Level Alignment and Quantum Transport

Theoretical modeling of electron transport across metal-molecule interfaces is a cornerstone of computational nanoscience of direct relevance to a number of fields including nano- and organic electronics, organic photo-voltaics, and electrochemistry. The theoretical description of quantum transport in molecular junctions has been a long-standing challenge which has been addressed using density functional theory (DFT) in its groundstate and time-dependent forms. This approach is known to suffer from several problems, mainly related to its inability to correctly describe energy gaps and level alignments of molecules at surfaces, but so far no better alternative has been available.

I will discuss our recent implementation of the GW method within a real space (localized atomic orbital basis) Projector Augmented Wave method, and show results for the ionization potential of isolated molecules as well as for the quantum conductance of metal-molecule-metal junctions.

Particular focus will be put on the important role of self-consistency in the GW self-energy. We find that the GW approximation significantly improves the DFT results both for the energy gaps, the level alignment, and the electrical conductance. In particular, dynamical screening effects in the substrate can shift the molecular levels be several electron volts substantially influencing both level alignment and conductance. Finally, some consequences of substrate-induced screening for the optical properties of adsorbed molecules will be discussed.

References:
Phys. Rev. Lett. 102, 046802 (2009)
Phys. Rev. B 80, 245427 (2009)
Phys. Rev. B 81, 085103 (2010)

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A-1040 Wien, Wiedner Hauptstaße 8-10