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

Dott. Angelo Valli

Institute of Solid State Physics, Vienna University of Technology, Austria

Dynamical vertex approximation for nanoscopic systems

At the nanoscale, both geometrical confinement and the reduced dimensionality enhance the effects of strong correlations between electrons. Dynamical Mean Field Theory (DMFT), based on the mapping of the lattice problem onto an effective quantum impurity model, revealed itself as a quite successful tool to deal with strongly correlated systems in the thermodynamic limit. We present a general scheme for the calculation of a finite-size complex network in the spirit of the recently introduced Dynamical Vertex Approximation, an extension of DMFT. For a benzene ring, we validate our approximation, at the single-particle level, against a numerically exact Quantum Monte Carlo solution for a multi-site Anderson Impurity Model. We propose a model for a quantum point contact made out of about a hundred correlated atoms. In agreement with experimental evidence, we observe a sharp drop of the conductance through the junction, which originates from a local Mott-Hubbard crossover. Further improvements are planned: including non-local correlation, i.e. extending the computation to the two-particle level, and studying real material through an interface with ab-initio calculation.

Date: Monday, Oct 25, 2010 16:00

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