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Self-Consistent Green's Function Embedding based on a Dynamical Mean-Field Concept

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In this talk I introduce an embedding scheme for periodic systems, the Real-Space Dynamical Mean-Field Embedding (RDMFE)[1], that facilitates a self-consistent treatment of the physically important part of a system with electronic structure methods, that are computationally too expensive for periodic systems. I use dynamical mean-field theory[2] (DMFT) to couple to the rest of the system, which is treated with less demanding approaches such as Kohn-Sham density functional theory. In contrast to the original DMFT formulation for correlated model Hamiltonians, I consider here the unit cell as local embedded cluster in an *ab initio* way, that includes all electronic degrees of freedom. The performance of my scheme is demonstrated by treating the embedded region with hybrid and *GW* self-energies (sc*GW*) for simple bulk systems. The total energy and the density of states converge rapidly with respect to the computational parameters and approach their bulk limit with increasing cluster size. For non self-consistent *GW* calculations a Plasmon satellite for Si is observed – in good agreement with periodic G_0W_0 calculations[3] - that vanish at self-consistency. The RDMFE@sc*GW* gap of 0 .9 eV for a two atom unit cell agrees well with previous G_0W_0 calculations and experiment. The same is true for the RDMFE@sc*GW* band structure.

The Analysis I present in this talk reveals that RDMFE has the potential to make advanced electronic methods accessible for unprecedented system sizes offering a multitude of application possibilities. The RDMFE scheme is thus a significant step towards making highly accurate theoretical approaches applicable to large systems.

[1] W. Chibani *et al.* PRB (2016)

[2] A.Georges *et al.*, Rev.Mod.Phys. (2006)

[3] M.Guzzo *et al.*, PRL (2011)

Biography:

Wael Chibani is a theoretical Physicist with a Master/Bachelor from the Technical University of Munich and a PhD in theoretical computational physics. Got PhD after a 4 years and 6 months stay at the Fritz-Haber Institute of the Max-Planck Society in Berlin, where he worked with the group of professor Matthias Scheffler on a novel embedding scheme based on Green functions following a dynamical mean-field concept. After the defense, worked for 6 months on a project part of the Novel Materials Discovery (NoMAD) Laboratory. After that moved to industry to work as a Consultant at Planisware Deutschland GmbH.