O 53: Invited Talk (Alexandre Tkatchenko)

Time: Wednesday 15:00–15:45 Location: TRE Phy

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The Many-Body Path Towards Quantitative Modeling of Complex Adsorption Systems — •Alexandre Tkatchenko — Fritz-Haber-Institut der MPG, Berlin, Germany

Reliable (accurate and efficient) modeling of the structure, stability, and electronic properties of complex adsorption systems remains a daunting task for modern electronic structure calculations. In the context of approximate density-functional theory, two thorny issues prevent us from reaching the goal of quantitative predictions: the (in)famous self-interaction error and the lack of reliable methods for an accurate description of van der Waals (vdW) interactions for hybrid organic/inorganic systems (HIOS). Both issues arise from the complexity posed by many-electron quantum mechanics, thereby demanding effective and novel solutions. Focusing on the role of vdW interactions, our recent developments of approximate many-body methods will be discussed along with a few surprises we found when applying these methods to HIOS: (1) The vdW energy can contribute more to the binding of covalently bonded systems than it does for physisorbed molecules; (2) the physically bound precursor state for aromatics on Pt(111) can be more stable than the corresponding chemisorbed state; (3) many-body vdW interactions lead to a binding energy for a fullerene molecule adsorbed on multi-layered graphene that *decreases* as a function of the number of underlying graphene layers. Finally, we discuss the challenges that lie ahead on the curved path towards fully quantitative many-body modeling of complex adsorption systems.