**Modeling Dielectric Response for Accurate Adsorption Energies**

**Jianmin Tao and Andrew M. Rappe**

Department of Chemistry, University of Pennsylvania

**ABSTRACT**: Many processes of technological and fundamental importance occur on solid surfaces. Adsorption is one of them that has received the most attention. In recent years, due to the rapid development of van der Waals (vdW) theory within the density functional formalism, much progress has been made toward fundamental understanding of this phenomenon. In this talk, I will first give a general description of adsorption. Then I will discuss the calculation of vdW coefficients between particles and surfaces by modeling dielectric response of particles and bulk solids [1,2]. This may serve as a dispersion correction to density functional approximations. Next, I will discuss sveral applications of accurate simulation of adsorption energies for atoms on transition metals, by incorporating the vdW interaction into the framework of density functional theory. Finally, a conclusion will be made.

References

1. J. Tao, J.P. Perdew, and A. Ruzsinszky, PRB **81**, 233102 (2010); PNAS **109**, 18 (2012).
2. J. Tao and A.M. Rappe, PRL **112**, 106101 (2014).