Theory and results of modeling van der Waals interactions in DFT

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In this seminar, I will start out by giving a general introduction of van der Waals interactions and their paramount importance in materials science. I will then outline the difficulties in reliably capturing them with common electronic structure modeling techniques and describe some widely used approximations within density functional theory (DFT). I will then focus on the details of vdW-DF, a non-local exchange-correlation functional that includes van der Waals interactions in a seamless fashion, sketching its history and derivation. Finally, I will present results for vdW-DF calculations on a wide variety of different systems, including water, physisorption/ diffusion/catalysis in metal organic framework materials, biomolecules and drug development, and hydrogen storage. Even though these systems are vastly different in nature, vdW-DF shows very encouraging results throughout. Where appropriate, I will compare our results with high-level quantum-chemistry calculations and point out strengths and weaknesses of the vdW-DF approach.

Dr. Thonhauser received his PhD in solid-state physics from the Institute for Theoretical Physics, Karl–Franzens–Universität Graz, Austria in 2001. He subsequently held Postdoctoral Research positions in the Department of Physics at The Pennsylvania State University and Rutgers University, followed by a Research Associate position at the Department of Materials Science and Engineering at the Massachusetts Institute of Technology. In 2008, Dr. Thonhauser joined the faculty in the Physics Department at Wake Forest University and meanwhile was promoted to Associate Professor with Tenure. His research is devoted to the application of condensed-matter theory to currently outstanding problems in physics, biophysics, chemistry, and materials science, with applications to nano-, bio-, and energy-related materials.