

Materials Science and Technology Division

**“A van der Waals DFT Approach
to Modeling Water”**

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Monday, September 28, 2009
11:00 a.m.
4500S, A-177

Abstract:

We will discuss our recent work in electronic-structure theory, which allows us to more accurately study water from first-principles. First, we will address a shortcoming of standard density functional theory, which gives poor results for systems with van der Waals interactions such as bulk water. To remedy the situation, we will discuss an exchange-correlation functional that includes van der Waals interactions in a seamless manner. The main advantage of our approach is the much more favorable scaling of the computational expense compared to standard quantum-chemistry approaches. We will also present a very efficient method to implement the aforementioned correlation-exchange functional. Second, we will discuss a Wannier-function approach to derive a fully quantum-mechanical theory for the orbital magnetization in periodic crystals, and subsequently, a novel way to calculate NMR chemical shieldings based on this new theory. Instead of obtaining the shieldings from the response to an external magnetic field, we derive it directly from the orbital magnetization appearing in response to a microscopic magnetic dipole. Finally, we show how the combination of NMR and van der Waals DFT can be applied to the study of water dimers and bulk water.

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