UW MRSEC
Interdisciplinary
Computational
Group

"PREDICTIVE THEORY OF ELECTRONIC STRUCTURE: ARE WE THERE YET?"

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When:	**Monday, March 10th, 2014 3:00 pm**
Where:	**Room 9341 Chemistry**
Host:	**Prof. Qiang Cui, Chemistry Department**

ABSTRACT:
Despite the stunning improvement of our ability to model chemistry computationally, the question remains: will we be able to predict — rather than rationalize — experimental outcomes in the foreseeable future? To predictively answer even basic questions relevant to chemists (what's the energy of a chemical bond? what's the activation energy of a reaction? how strong is a van der Waals force?) we must be able to describe surprisingly subtle changes in the electronic structure, with unprecedented precision. Here I will describe how the challenge of predictive simulation can be met, what the current roadblocks are, and the recent work to make possible electronic structure computation of "predictive" quality on hundreds of atoms.

This is a joint seminar between UW MRSEC Interdisciplinary Computational Group and the Theoretical Chemistry Institute (TCI) at UW-Madison.