

**Friday, October 23, 2015  
4:10 – 5:00 PM  
EPS103**

**The role of an accurate description of local structure to inform our understanding of nucleation and assembly in the condensed phase**

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[http://www.pnl.gov/science/staff/staff\\_info.asp?staff\\_num=5981](http://www.pnl.gov/science/staff/staff_info.asp?staff_num=5981)

<http://ms3.pnnl.gov/default.aspx?topic=Christopher J. Mundy>

**Abstract:**

A challenge in materials science is how to utilize information from a molecular simulation to build a quantitative model of solution phase nucleation and assembly. I will make the case that an accurate description of local aqueous structure, as verified by experiment, is imperative in order to describe long-range collective response. We use the tools of statistical mechanics and molecular simulation (classical and quantum) to construct reduced models of interaction based on the principle of solvent response to interfaces. This provides a link from molecular scale descriptors to macroscopic outcomes.

**Host: Hugo Schmidt, Department of Physics, Pat Callis, Department of Chemistry, Rob Walker and Erik Grumstrup, Department of Chemistry and MUS Materials Science Ph.D. Program**

**\*\*\* Refreshments served in the EPS second floor atrium at 3:45 \*\*\***