UW MRSEC
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Group

"DEVELOPMENT AND APPLICATION OF AB INITIO FORCE FIELDS FOR ORGANIC AND IONIC LIQUIDS"

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(in collaboration with Prof. JR Schmidt and Prof. Arun Yethiraj)

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When:	**Monday, February 2nd, 2015 3:30 pm**
Where:	**Room 1153 Mechanical Engineering Building**
Host:	**Prof. JR Schmidt, Chemistry Department**

ABSTRACT:
In this seminar, we will discuss how perturbation theory (namely *symmetry-adapted* perturbation theory) can be used for 1) accurately describing the intermolecular interactions determining the properties of bulk liquids and 2) as a framework for developing transferable, atomistic force fields for these systems. We will outline the basis of our force-field development methodology, relying on the expression of asymptotic intermolecular interactions between molecules strictly in terms of monomer properties, and subsequently modeling these monomer properties using transferable, atomistic parameters. Finally, we will demonstrate that by incorporating all relevant components of the leading two- and three-body intermolecular interactions, we can accurate predict the properties of both "weakly" interacting organic liquids and "strongly" interacting ionic liquids entirely from first principles.