Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

**Applications of a novel QM/MM method incorporating a polarizable force field.** CHRISTOPHER WILLIAMS, JOHN HERBERT, Ohio State University — In conventional QM/MM methods the MM region is modeled by a force field that uses a set of point charges to represent the electrostatics. However, recently developed force fields use multipole expansions combined with polarizable sites to to represent electrostatic interactions. A novel algorithm is presented to interface this class of force fields with a QM region by allowing the QM region and the MM region to polarize each other self-consistently. It is implemented using the QChem electronic structure code and the AMOEBA force field as implemented in the software package TINKER. The algorithm is general and can be used with a variety of QM methods including MP2 and DFT. Examples of both ground state and excited state calculations are presented, including the investigation of the effectiveness of many-body expansions in modeling the solvation of charged species and the effect of charged environments on biomolecules.

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Date submitted: 21 Nov 2008 Electronic form version 1.4