Abstract for an Invited Paper
for the MAR07 Meeting of
The American Physical Society

QM/MM in complex systems using SCC-DFTB and its implementation in Amber.

ADRIAN ROITBERG, University of Florida

We will present our current implementation of SCC-DFTB into the molecular dynamics program Amber. Details of the efficiency and accuracy of the method will be presented. We will also shows some case studies involving conformational searches in peptides, replica exchange simulations in solution, and an application to an enzyme mechanism.