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Beyond force fields. QM/MM conformational searches in biomolecules using Replica Exchange molecular dynamics.

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Force fields have been extremely successful for our understanding of structure, energetics and dynamics of biomolecules. However, they neglect, for the most part, quantum effects such as charge transfer and polarization. In this talk I will present our work using our newly developed QM/MM interface in the program Amber, which can very efficiently treat small peptides in explicit solvent using a number of different semiempirical methods. We use Replica Exchange molecular dynamics to sample the surface properly and ensure convergence. A comparison of the conformational space sampled by different semiempirical methods in explicit water classical models will be presented. The computational results will be compared against NMR experiments.