

Applications of the Amber/PUPIL interface for hybrid QM/MM calculations

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PUPIL (Program for User Package Interfacing and Linking) is a free, open source, Java-based system for the interfacing of general molecular mechanics (MM) and quantum mechanics (QM) programs in a single multi-scale simulation, with or without source-code access to the QM program.

The implementation allows a driver MM program (Amber, for example) to obtain energies and forces for a subset of the atoms from a QM program (such as Gaussian or NWChem) for a hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) simulation. This use of a separate QM program allows access to a much greater range of QM methods than conventional QM/MM implementations, while the specialized techniques from the driver program (umbrella sampling, multiple steering MD, etc.) are still available.

In this presentation, we will show diverse applications of the Amber/PUPIL interface with a number of external QM programs. We will present umbrella sampling and MSMD (Jarzynski) simulations, carried out using Amber in combination with the Gaussian03 QM program, as well as examples involving other QM programs.

