The Development of Accelerated Quantum Molecular Dynamics for Complex Gas-Phase Reactive Systems

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A suite of programs called **A**ccelerated **Mol**ecular **D**ynamics with **C**hemistry (*AMolDC*) has been written, tested, and employed in order to perform time-dependent, multilevel QM/MM simulations.

Demonstrated results:

-Very accurate interpolations for very large and diverse chemical systems including saturated and unsaturated hydrocarbon rings and chains that contain a variety of functional group moities.

-Integrated interpolation module yields orders of magnitude reduced computational costs compared to parallel QM calculations.