Abstract

Title: A QM/MM Study of Host-Guest Interactions

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The molecular mechanics-based chemistry package VeraChem has been interfaced with the ab initio quantum chemistry package GAMESS in order to predict binding free energies of host-guest complexes more accurately. Molecular geometries were optimized using quantum mechanical methods. The computational cost is usually time intensive due to the large number of geometry optimizations of potential conformers. However, a progressive scheme was recently introduced and implemented in the VeraChem software package to mitigate this problem by checking the energy and gradient during geometry optimization and eliminating structures that would not result in low-lying minima on the potential energy surface. Preliminary testing showed that the computational time has reduced significantly without loss of accuracy.