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Investigating Potential Surfaces with QM/MM Methods

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Geometry optimization of large QM/MM systems is not trivial, especially when transition states or higher order saddle points are desired. The optimization can be carried out with a macro/micro scheme, which alternates (internal coordinate) geometry steps in the QM region with full (cartesian) minimizations of the MM region. This significantly reduces the number of QM calculations, and avoids bottlenecks associated with coordinate transformation and Hessian manipulation. This standard macro/micro scheme, however, suffers from numerical instability and compromised convergence behavior. This affects particularly the optimization of transition states, which is therefore not often successful. To address these problems we present extensions to the macro/micro scheme, which have been implemented in the ONIOM framework for hybrid methods. In the standard scheme, the QM and MM regions are coupled only through first order terms. We now include second order coupling using analytical MM contributions, employing linear scaling methods. We show how this improves convergence and allows for the optimization and characterization of saddle points in very large systems. We demonstrate our methods using various examples, such as the hydrogen peroxide reduction by Selenoprotein Glutathione Peroxidase, proton transfer in H-Y zeolite, and thermal isomerization of retinal in Bacteriorhodopsin.