

New transformation matrix and analytic MP2 gradient of the GHO QM/MM method

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We have developed QM/MM methods based on the generalized hybrid orbital method (GHO)¹. In the GHO method, sp^3 hybridized orbitals are generated and used for each boundary atom of QM and MM. In our latest development, we have improved the accuracy of the GHO method by introducing a new transformation matrix assuming that all the coefficients of p -hybridized orbitals are uniform and each hybridized orbital points toward a vertex of a tetrahedron. Moreover, we have developed analytic energy gradient of GHO-MP2. We will show some numerical results of the new implementation for some systems involving alanine dipeptide and c-AMP dependent protein kinase (PKA).

Reference

1. Jaewoon Jung, Cheol HO Choi, Yuji Sugita and Seiichiro Ten-no, "New implementation of a combined quantum mechanical and molecular mechanical method using modified generalized hybrid orbitals", J. Chem. Phys., **127**, 204102 (2007)