2P02

New implementation of QM/MM methods using modified generalized hybrid orbitals (GHO)

J. Jung[1], C.-H. Choi[2], Y. Sugita[3], and S. Ten-no[1]

1. Graduate School of information Science, Nagoya University, Nagoya, Japan
2. Department of Chemistry, Kyungbuk National University, Tae-gu, South Korea
3. RIKEN, Tokyo, Japan

E-mail : jwjung@info.human.nagoya-u.ac.jp

We develop novel QM/MM methods based on a frozen orbital treatment named the generalized hybrid orbitals (GHO). In the GHO method, sp^3 hybridized orbitals are generated for each boundary atom. One of them is used as an active orbital quantum mechanically and the rest three are used as frozen auxiliary orbitals. The original GHO method parameterizes the occupation numbers of auxiliary orbitals only from the partial charges of boundary atoms. The occupation number assigned to each auxiliary orbital is chosen to be $1-\frac{q_B}{3}$, where q_B is the MM partial charge of the boundary atom, so that the charge is equally distributed over the three auxiliary orbitals.

In our new implementation, all MM atoms linked to the boundary atoms are taken into account. First, the occupation numbers of auxiliary orbitals are determined according to the electronegativity of the neighboring MM atoms. Then, the occupation numbers are modified according to the neutrality condition of the boundary atom and MM atoms that are linked to the boundary. In addition, we introduce an ortogonalization procedure among the auxiliary orbitals of different boundary atoms. The original GHO method assumes that the overlaps between different auxiliary orbitals are zero. Nevertheless there are overlaps between different auxiliary orbitals in reality if there are more than two boundary atoms. In this case, we make a Lowdin orthogonalization procedure among auxiliary orbitals.

We have implemented the analytic gradient method based on the new GHO energy functional. The performance of the method will be discussed in detail.