QM/MM Border Region Treatment: Recent Improvements

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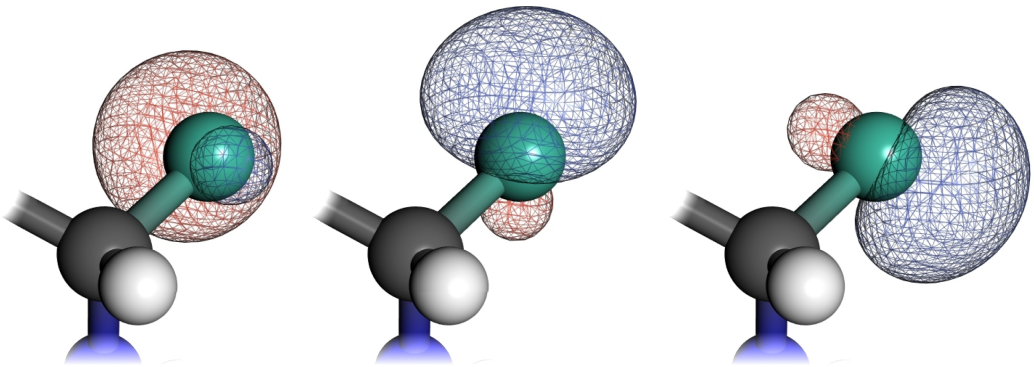
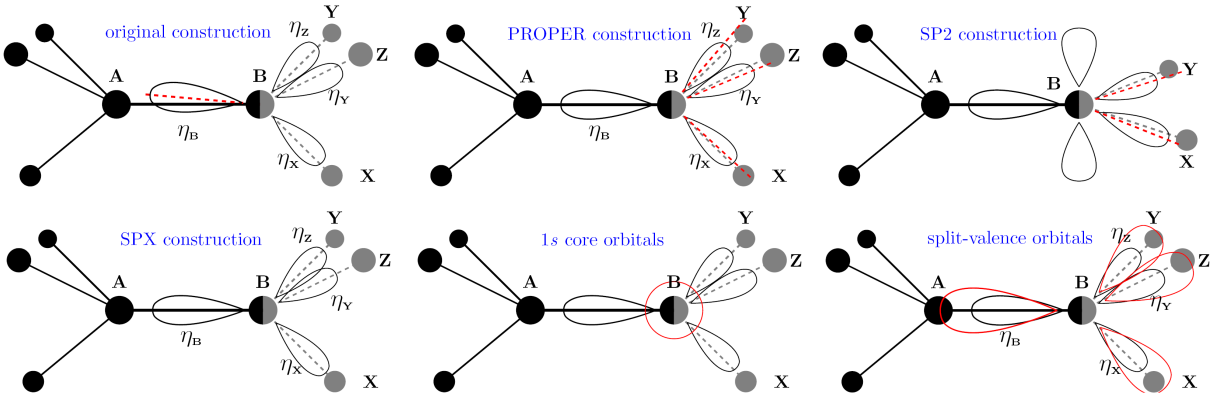
The improvement of saturation methods for use in the QM/MM field of research is an ongoing process, motivated by the fact that better saturation leads to smaller quantum-chemical surroundings which in turn leads to less computational cost. We present here our recent developments in the Generalized Hybrid Orbitals method introduced by Pu, Gao and Truhlar. [1]



A year ago, we published a summary of our developments.[2] We could show that using more sophisticated construction methods for the hybrid orbitals, relocating the MM partial charge of the GHO atom and including both core orbitals and higher orbital shells lead to strong improvements in the calculated results. In all cases, the GHO atoms surpass the saturation with hydrogen atoms.



Recent developments have lowered the error introduced by the GHO atom even further and show the expected behaviour for increasing complexity of the construction method. The SPX construction using the actual geometry of the MM atoms gives the best results, taking into account the specific environment of the GHO atom. We were also able to do calculations with the 6-31G basis set showing the effect of higher basis sets on GHO atoms compared to the STO-3G basis set. Here, it can also be seen that using those split-valence basis sets *without* the 1*s* core orbitals leads to very strong deviations. It is therefore recommended to use those two options together.

[1] J. Pu, J. Gao, D. G. Truhlar, *JPhysChemA*, **2004**, *108*, 632-650.
[2] S. M. Eckard, T. E. Exner, *IntJQuantChem*, **2009**, *109(7),* 1451-1463.