Minimum-Energy Conical Intersection optimization with Double Newton-Raphson Algorithm inside ONIOM Scheme

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The Double Newton-Raphson (DNR) is a new algorithm to found Minimum-Energy of the Conical Intersection (MECI) that improve the results of the old algorithms – it needs less steps and obtain better degenerations and minimums. MECI are important point inside the potential energy surface (PES) that help to understand the photochemistry and photo-physics process of lots of components. A special case of this are DNA or other big biomolecules where the QM calculations are extremely expensive. The unique way to calculate this biomolecules with good accuracy is with QM/MM methods. The ONIOM scheme is a very popular QM/MM method implemented in Gaussian by Prof. Morokuma[1] [2]. Following this idea, we implement DNR algorithm with ONIOM scheme to calculate MECI of a big biomolecules like DNA.

In the presentation, we explain the theory of DNR inside ONIOM, how the implementation is done inside Gaussian code and compare DNR inside ONIOM with the old algorithms inside ONIOM.

1 S. Dapprich, I. Komáromi, K. S. Byun, K. Morokuma and M. J. Frisch, *J. Mol. Struct.,* 462, **1999**

2 T. Vreven, K. S. Byun, S. Komáromi, S. Dapprich, J. A. Montgomery, K.Morokuma, M. J. Frisch, *J. Chem. Theory Comput.*, **2006**, 815