Development of Multistructural Microiteration Technique and its Application to Enzymatic Reactions

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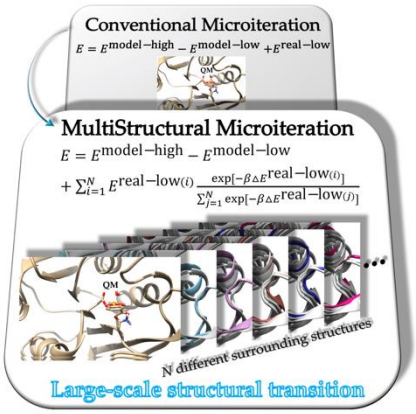
Abstract: We have proposed a technique called the multistructural microiteration (MSM). [1-3] MSM describes the structure of the MM part as the average of multiple surrounding structures and takes account of their contributions during geometrical optimization and reaction path calculations as shown in Figure. This technique is just a simple extension of QM/MM-ONIOM method, and the computational cost is comparable to that of conventional one. Despite the simplicity, MSM has been successful in describing large-scale surrounding structural transitions such as from open- to closed-loop conformation and *vice versa* during chemical reactions.[2] Recently, we combined MSM with the electrostatic embedding (EE) scheme of the QM/MM-ONIOM method by extending its original formulation for mechanical embedding (ME). From test calculations, numerical results of MSM-EE yielded barriers and reaction energies close to experimental values with computational costs comparable to QM/MM-ONIOM-ME or -EE methods. In this presentation, we will show the details of MSM algorithm and its applications.



[1] **K. Suzuki**, K. Morokuma, and S. Maeda, *J. Compt. Chem.*, **38**, 2213 (2017).

[2] **K. Suzuki**, S. Maeda, and K. Morokuma, *ACS Omega*, **4**, 1178 (2019).

[3] **K. Suzuki** and S. Maeda, *Phys. Chem. Chem. Phys.* **24**, 16762 (2022).