Automated Reaction Path Search by the Artificial Force Induced Reaction Method

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The mechanism of chemical reactions can be studied by calculating reaction paths based on quantum chemical calculations. The intrinsic reaction coordinate (IRC), which is the steepest descent path (in the mass-weighted coordinate) from the first-order saddle point, is often calculated as a reaction path. A chemical reaction can thus be predicted once all the first-order saddle points relevant to the reaction are obtained. However, it is not feasible to explore the entire configurational space of molecules of practical sizes. On the other hand, since the reaction path is a one-dimensional line, it is ideal if the reaction path can be searched by tracing the reaction path itself. However, it was shown that it is impossible to trace IRCs from a local minimum to another local minimum.

We have tried to approach the ideal of finding a reaction path by following a reaction path by proposing approximate reaction paths that can be traced from a local minimum. The artificial force induced reaction (AFIR) method pushes (or pulls) reaction sites to each other, to find approximate reaction paths [1]. The AFIR method has been applied to many organic reactions and photoreactions. In this presentation, the AFIR method implemented in the GRRM program is introduced [2].

The algorithm of the AFIR method is simple enough to be applied even to complex reaction systems. Therefore, generalization to various reaction systems as shown in Fig. 1 has been realized. For example, we have recently reported the automated construction of reaction path network for surface reaction shown in Fig. 2 [3]. These latest developments will also be discussed.

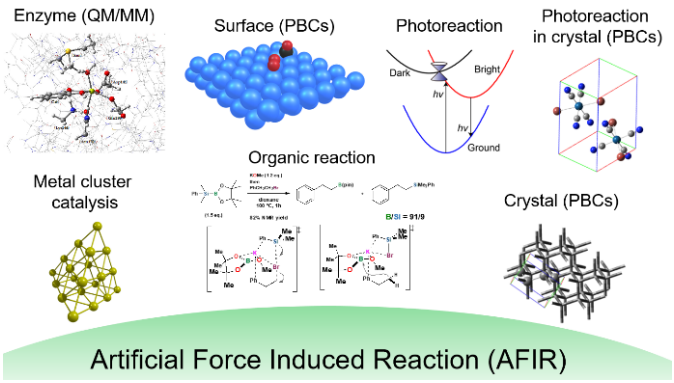

Fig. 1. Application scope of the AFIR method.

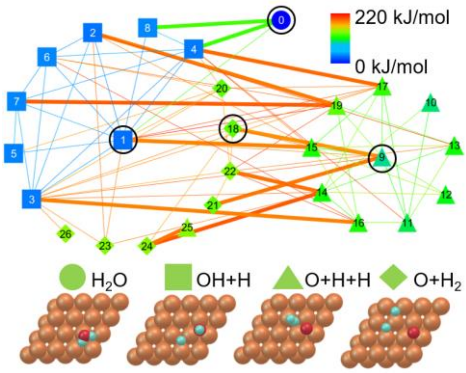

Fig. 2. Reaction path network of H_2O on the Cu(111) surface [3].

Bibliography

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[3] S. Maeda, K. Sugiyama, Y. Sumiya, M. Takagi, K. Saita, *Chem. Lett.* **2018**, (in press).

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