Accelerating efficient reaction path search using NNP-AFIR method by pre-trained models

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Automatic reaction path search by NNP-AFIR method is efficient for systematic exploration of global potential energy surfaces, with DFT-level accuracy at semi-empirical cost, but need new a model for each system. To further decrease the cost, we developed a transferable pre-trained model which can be applied to various systems after minimal fine-tuning, enabling high-throughput mechanism analysis.

Starting from a minimal system (3 C_2H_2 + 2 H_2O + 2 NH_3), AFIR searching was used to construct a reaction network of high diversity for CHNO systems. This dataset includes transition states from over 100 reaction types and rich atomic environments, resulting in a model with strong robustness and transferability. Following tests on an aromatic Passerini reaction system away from training domain proved that NNP-AFIR with this model successfully identified the final product and the multi-step reaction pathway, with 14 kJ/mol MAE over more than 20,000 structures even without fine-tuning. The computational efficiency of NNP-AFIR in organic systems is therefore improved.

Using our robust pre-trained model with subsequent light fine-tuning, we further reduce the computational cost of NNP-AFIR for organic systems, providing a powerful framework for accelerating the rational design of novel reactions by tackling more complex systems.