Evaluation of synergistic effects in chemical reactions of multinary systems and its application to catalyst development

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Brief overview

The aim of this project is to establish methods to predict the reaction indices like adsorption and activation energies, to specify their origins, and to evaluate the synergistic effects in chemical reactions of multinary systems by constructing database of the results of electronic structure calculations and experiments and cooperatively applying the data scientific methods. The fruit of this project will significantly improve the throughput of catalyst development, as well as elucidate the synergistic effects of multinary systems appearing in various chemical phenomena.

Achievement

Targeting to the metal nanocluster catalysts, we successfully specified the main factor for the catalytic activity (Fig. 1) and predicted the adsorption and activation energies (Fig. 2) by constructing the database of the reaction paths and transition states obtained by, for example, GRRM, an automatic reaction path search program. We also constructed the electronic structure database of surface molecular adsorption systems for analyses of heterogeneous catalytic reactions. By the data analysis combined with experimental database, we predicted the catalytic activity for the methane steam reforming.

Fig. 1.

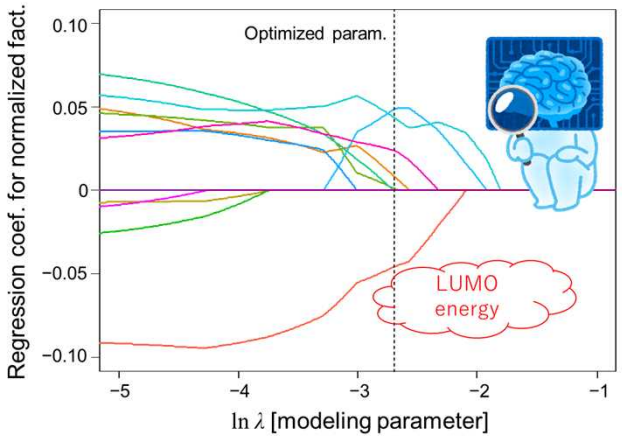
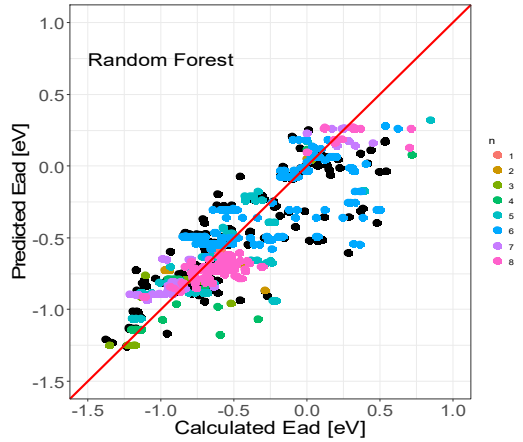


Fig. 2.



Reference/Link

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