Perspectives in catalysis on modeling the reactivity of active sites

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Abstract

Since the discovery of active sites by Sir Hugh Taylor, researchers in catalysis are intrigued by the identification and nature of atomic sites which actively participate in turning over the catalytic cycle. For decades, heterogeneous catalysis is considered to be functioning at the most stable sites on the catalyst surface, wherein the elementary reactions are bound to follow a unique linear relationship between the reaction and activation energies. However, in an altered paradigm, the reactivity of single atom alloys is showing a breakdown from linear scaling [1], leading to erroneous interpretations from a first principle microkinetic model, employing scaling relations and machine learning tools [2, 3]. Moreover, the site itself may not be the sole contributor of reactivity. Instead, a statistical ensemble of active sites which could include the reactivity of metastable species, may provide a more-suited expression for reaction rates. This is elucidated in the reactivity of metastable molybdenum carbide nanoclusters for C-H activation in alkanes and alkenes [4]. Overall, the evolved understanding of active site is providing a unique opportunity for rational catalyst design.

References

1. Iyer, J., Jalid, F., Khan, T.S. & **Haider, M. A.** (2022): *Reaction Chemistry and Engineering,* 7, 61-75.
2. Kumar, A., Iyer, J., Jalid, F., Ramteke, M., Khan, T.S. & **Haider, M. A.** (2022): *ChemCatChem, 14*, e202101481.
3. Saxena, S., Khan, T. S., Jalid, F., Ramteke, M. & **Haider, M. A.** (2020): *Journal of Materials Chemistry A*, 8(1), 107–123
4. Balyan, S., Saini, S., Khan, T. S., Pant, K. K., Gupta, P., Bhattacharya, S. & **Haider, M. A.** (2021): *Nanoscale*, 13(8), 4451–4466

Biosketch

Dr. M. Ali Haider is an Alexander von Humboldt fellow at the Catalysis Research Center of the Technical University Munich. He has completed his M.S. and Ph.D. in Chemical Engineering at the University of Virginia and B.Tech. from Indian Institute of Technology (IIT) Guwahati. He joined the Department of Chemical Engineering at IIT Delhi in 2013. He was a visiting scholar at the University of Delaware on a *'Bioenergy-Award for Cutting Edge Research'* sponsored by the Indo–US Science and Technology Forum. His research interests are focused on experimental and theoretical heterogeneous catalysis applied to renewable energy and chemicals. He has received '*Dr. A.P.J Abdul Kalam HPC Award for R & D in HPC Applications'* by Hewlett Packard Enterprise and Intel. Indian Institute of Chemical Engineers has bestowed him the '*Amar Dye-Chem Award for Excellence in Basic Research and Development in Chemical Engineering'*. He is a recipient of the '*DAE-BRNS Young Scientist Award'*, 'Gandhian Young Technological Innovation Award' and Institution of Engineers (India) '*Young Engineers Award'*. Journals of the Royal Society of Chemistry have recognised his contributions at various occasions as an *'Emerging Investigator'*, *'Highly Cited Author'* and in *'Editor's Choice Collection'*. At IIT Delhi, his contributions in teaching and research are noted by the *'Industry Relevant Best PhD Thesis Supervision'*, *'Teaching Excellence Award'* and *'Early Career Research Award'*.