Tata Institute of Fundamental Research
Survey No. 36/P, Gopanpally Village, Serilingampally, Ranga Reddy Dist., Hyderabad – 500 046

Internal Seminar

Probing mechanisms of homogeneous catalysts with density functional theory

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Homogeneous catalysis has played a pivotal role in the advancement of chemical synthesis, providing a powerful means to achieve chemical transformations that were once considered chemically inert.[1,2] With the use of first row transition metals, various chemical transformations, such as C-C coupling reactions, CO_2 reduction, and activation of inert C-O bonds in lignocellulosic biomass, have become possible under catalytic conditions.[2,3] First row transition metals offer several advantages, including high abundance on earth, low cost, low or no toxicity, and unique catalytic characteristics. Computational methods like Density Functional Theory (DFT) provide an effective way to understand the mechanistic details of the catalytic cycles, which can aid in the design of better catalysts for sustainable chemical synthesis.[4]

References:

(1) Kumar, A.; Daw, P.; Milstein, D. Homogeneous catalysis for sustainable energy: Hydrogen and methanol economies, fuels from biomass, and related topics. Chem. Rev. 2021, 122, 385-441.
(2) Su, B.; Cao, Z.-C.; Shi, Z.-J. Exploration of earth-abundant transition metals (Fe, Co, and Ni) as catalysts in unreactive chemical bond activations. Acc. Chem. Res. 2015, 48, 886-896.
(3) Ragauskas, A. J.; Beckham, G. T.; Biddy, M. J.; Chandra, R.; Chen, F.; Davis, M. F.; Davison, B. H.; Dixon, R. A.; Gilna, P.; Keller, M. Lignin valorization: improving lignin processing in the biorefinery. Science 2014, 344, 1246843.
(4) Ahn, S.; Hong, M.; Sundararajan, M.; Ess, D. H.; Baik, M.-H. Design and optimization of catalysts based on mechanistic insights derived from quantum chemical reaction modeling. Chem. Rev. 2019, 119, 6509-6560.

Thursday, Mar 28th 2024

11:30 Hrs

Auditorium, TIFR-H