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How to design a bi-functional molecular catalyst for hydrogen production from methanol?

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Abstract (not more than 300 words)

We have studied the mechanism of hydrogen production from methanol by two different, and well known ruthenium based molecular catalysts: Ru(trop)$_2$dad [1,2] complex, and pincer supported Ru-PNP [3] complex using Density functional theory (DFT), in conjunction with *ab initio* molecular dynamics studies (AIMD) with explicit solvation. The results show that while methanol dehydrogenation occurs via a Noyori type (Ru - N) bi-functional mechanism by the Ru(trop)$_2$dad catalyst, the RuPNP complex does not feature the commonly assumed (Ru - N) bi-functional mechanism under the applied reaction conditions. Ru(trop)$_2$dad catalyst does not require any additive (base/Lewis acid) for activity while the RuPNP complex requires 8M KOH for optimal activity. Several other well-known molecular catalysts also require an additive (base/Lewis acid) for hydrogen production from methanol. Therefore, the mechanistic studies on Ru(trop)$_2$dad and RuPNP systems, and the sharp contrast in their respective mechanistic pathways, provide guidelines for rational design of additive free and highly active bi-functional catalysts for hydrogen production from methanol. Moreover, these case studies show the importance of an explicit consideration of solvent molecules for realistic computational modelling of minimum energy reaction pathway.

Keywords— *bi-functional catalysis, ab inito molecular dynamics, Density Functional Theory, additive-free methanol dehydrogenatio*n

Professional Biography (100-150 words)

Vivek Sinha completed his Integrated BS-MS in Physical Sciences at the age of 23 from the Indian Institute of Science Education and Research, Kolkata. He is currently a final year PhD researcher at the University of Amsterdam in the Shell-NWO Computational Science for Energy Research (CER) program. His research primarily focuses on using Computational Chemistry to understand hydrogen generation from simple molecules, and rational design of molecular catalysts.



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