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Computational study of electrochemical reduction of CO_2 on transition metal/p-block nanocatalysts

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Nanocatalysis, the study of catalysts for various homogeneous and heterogenous industrial applications is a vastly researched field these days. Factors such as depleting fossil fuels, increasing fuel costs and rising CO_2 emissions are some of the major reasons for the need to research on promising (efficient and sustainable) catalyst technologies. Electrochemical reduction of CO_2 using heterogenous catalysis is one of the solutions to convert CO_2 to value added hydrocarbon fuels which can later be used in various industrial applications like fuel cells. Developing a non-precious catalyst with high energy efficiency which can reduce the overpotential without compromising with the performance of the catalyst and selectivity of the products is a major challenge. Till date, Copper is the only effective catalyst which can reduce CO_2 to hydrocarbons such as methane and methanol. Our work mainly focuses on computationally screening different nanocatalysts for CO_2 electroreduction. In particular, we study transition metal/metal oxides – p-block hybrids (non-precious metal catalysts) that can electrochemically convert CO_2 to value added fuels which can satisfy all or at least some the characteristics of an effective catalyst as discussed above. So far, we have studied WO_3, MoO_3, ZnO and ZnS surfaces for CO_2 electroreduction by generating various possible reaction pathways from CO_2 to CH_4 and CH_3OH. We use density functional theory, DFT calculations to find the adsorption properties of each intermediate species. These studies may not be enough to decide which is the best for CO_2 electroreduction, however, these will help in designing similar catalysts and can be a basis to do experimental study for the same process.

Biography

Sahithi Ananthaneni is currently a second year PhD student in Chemical Engineering at Villanova University, under the supervision of Dr. Rees Rankin. Her main research focus is in nanocatalysis. She works on the computational modeling and design of nanomaterials through DFT calculations, with the hope to use them for future catalytic applications. She has completed her Master's degree in Chemical Engineering from Villanova University in 2016. During her Masters, she has worked on two different projects focusing on nanoelectronics and nanocatalysis.

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