DESIGNING CATALYSTS FOR ENERGY INTENSIVE PROCESSES USING COMPUTATIONAL TECHNIQUES

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The significant challenge faced by our global society, from issues of climate change to question of energy security could be solved if we can find a champion catalyst that can convert atmospheric CO_2 to carbon based fuels. However, designing catalytic nanostructures that can thermochemically or photochemically convert gaseous CO_2 into fuels is a significant challenge which requires a keen understanding of the physical and chemical properties of complex materials and the processes happening on them at atomic and electronic level. In this context, I will present my recent findings in the area of gas phase heterogeneous catalysis achieved by using computational techniques in conjunction with experimental research. Specifically, in this talk I will highlight the insights provided by computational analysis into the surface chemistry of CO_2 reduction reaction on $In_2O_{3-x}(OH)_y$ nanoparticles, in the presence and absence of light and temperature, which resulted in the discovered of a new class of "frustrated Lewis pair" (FLP) heterogeneous photocatalysts. Further, I will discuss the challenges faced in commercializing the existing sustainable solutions for other energy intensive processes (such as generating electricity via polymer electrolyte membrane fuel cells, ammonia synthesis, and CO_2 capture) and how computational tools will be utilized to improve these processes in my future research work.