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 ammonia synthesis, generating electricity via polymer electrolyte membrane fuel cells and solid oxide fuel cells, etc.) and how computational tools will be utilized to improve these processes in my future research work.