University at Buffalo
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Ag ion-exchanged zeolites for hydrocarbons and nitrogen oxides trapping application

Stringent emission regulations led to significant attention for reducing vehicle emissions during the cold-start that takes place the first 1-2 minutes of vehicle operation [1]. A potential approach to regulate the cold-start emission is to utilize hydrocarbon (HC) and nitrogen oxide (NOx) traps. Zeolites have been emerged as potential trapping materials due to their tunable acidity, high surface area, and thermal stability [2]. In this work, a series of Ag containing ZSM-5 zeolites with different Ag loadings (5 - 4.6 wt.%) were prepared via ion-exchange. Their trapping performance was evaluated using a simulated diesel exhaust steam (900 ppm C2H4, 900 ppm C7H8, 100 ppm NOx, 12% O2,6% CO2, 6% H2O, 2000 ppm CO, 400 ppm H2). The adsorption of single HCs and NOx was also investigated. The results indicate that Ag is able to act as an adsorption site for both C2H4 and C7H8 in the presence of H2O. Increasing the Ag loading from 0.5 to 4.6 wt.% enhance the HC adsorption capacity, attributed to an increase in the number of adsorption sites. The oxidation state of Ag (e.g. Ag+, Ag0) influences the HC adsorption. Specifically, Ag+ shows higher adsorption efficiency (90%) in C7H8 compared to Ag0 (82%). This is attributed to the limitation of the π-backbonding between Ag0 (lack of empty orbital) and C7H8. Finally, durability of Ag/ZSM-5 was evaluated after hydrothermal aging at 800 oC for 10 h under 10% O2, 5% CO2, and 5% H2O. Our results showed that C2H4 and C7H8 adsorption capacity was maintained even after hydrothermal aging, indicating that Ag/ZSM-5 is thermally stable and suitable for trapping applications.

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Charge carrier transport in photocatalytic materials: Multiscale modeling and Application to bismuth vanadate BiVO4

The Holy Grail in efficient and cost-effective conversion of solar energy into electrical and chemical energy is solar energy-driven water splitting using semi-conductor-based photo-catalysts. Overall conversion efficiencies of best systems so far are however far from the level needed for practical applications. Viable materials must exhibit good *visible light absorption* and carrier generation, good *carrier transport*, and good *redox reactivity*. This presentation will focus on carrier transport studied by multiscale modeling, combining DFT+U calculations of polaron hopping by Marcus/Holstein theory and kinetic Monte Carlo (KMC) modeling of mesoscale transport. We will highlight the approach first for stoichiometric bulk $BiVO_4$ (BVO), the most promising anode material to date: e^- transport occurs via V-to-V through-space hopping while h^+ transport proceeds via through-space and through-bond hopping; h^+ transport is bi-modal, with fast transport-inefficient rattling hops within VO_4 tetrahedra, and slower transport-efficient hops across pairs of tetrahedra. [1] We will then present results for W/Mo-doped BVO. Each W or Mo doping atom contributes a mobile e^- that does not reside on dopant lattice sites. There exists a shallow region of attractive interaction around the dopant site extending to up to ~ 3 nearest neighbor shells. The increase in carrier density upon doping overshadows the marginal decrease in electron mobility in doped bulk BVO. [2] The electronic conductivity is shown to monotonically increase with increasing doping levels. We will show how the effect of shallow attraction regions is more appreciated through controlling the spatial distribution of doping concentrations towards enhanced charge carrier separation.

Wednesday Seminar Series