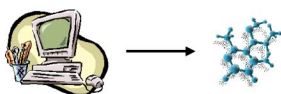


Investigator: Stan Zygmunt

My research is in the area of computational catalysis, which involves the calculation of the reaction pathways and energies of molecules interacting with catalytic sites.

I am currently studying the oxidative dehydrogenation (ODH) of the hydrocarbon molecule propane to propene using a vanadium oxide catalyst. This work shows that the ODH reaction is facilitated by a spin crossing from the singlet to the triplet state, which lowers the energy barrier for the reaction.



The PDF Footer