Abstract

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Title: Density Functional Theory Simulations of MOFs Encapsulated-Catalyzed Systems
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The research is mainly on Computational Design of Highly Selective Transition Metal Catalysts Encapsulated by Metal-Organic Frameworks for Butane Oxidation to 1-Butanol. Metal Organic Framework (MOF) grown over a heterogeneous catalyst. Pores of framework allow only certain molecules of correct size, orientation, or chemical properties to access catalyst. The framework will force molecule into desired orientation where only the terminal atoms will "see" the catalyst. In our simulation we would like to use the helium ring to simulate the MOFs pores, since He is inert and exhibits the no chemical reactivity. The reaction we are looking into is butane oxidation to 1-butanol. The specific catalyst surface, which we are working on, is Ag3Pd. However, we found that there is problem existing on the very first oxygen dissociation step which the activation energy and reaction energy is positive and pretty large. As a result, we are taking consideration into other Alloy surface such as Cu3Pd and PdZn , which bind the O2 more strongly and may facilitate the O2 dissociation. What's more, the metal oxide is another material we will look into in the future.

Reference:

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2. Getman, R. B., Schneider, W. F., Smeltz, A. D., Delgass, W. N., and Ribeiro, F. H. Phys Rev Lett 102, 076101 (2009