Title: Investigation of the Dehydration of 2-Propanol for NWChemEx

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Abstract:

NWChemEx contains an umbrella of modules that can be used to tackle most electronic structure theory calculations being carried out today. Electronic structure theory provides a foundation for understanding chemical transformations and processes in complex chemical environments. We are working on setting up measures for chemical systems embedded in a larger system. The zeolite case that we are interested in is an example of such a case. How does the zeolite structure affect the chemistry? Catalysts are the cornerstone of the chemicals industry, whose products are used in nearly all human endeavors. This work uses density functional theory (DFT) to understand how water is removed from organic compounds (2-propanol) to form new chemicals over H-ZSM-5 zeolite.

Our goals are to lay the groundwork for the mechanistic simulations and study the energy at different stages and transition states. Further insights into catalytic properties could be obtained by comparing DFT calculations to other corresponding methods of predictions. The studies presented here show how detailed electronic structure calculations can be used to develop a deeper understanding of catalysts, which might be improved. We aim to investigate the dehydration of 2-Propanol using NWChemEx. Our preliminary results show how the enthalpy of each basis set decreases as the number of valence orbitals increases. The poster presents the data of the dehydration of 2-propanol, propene, water, and enthalpy using five correlation-consistent basis sets: cc-pVDZ, cc-pVTZ, cc-pVQZ, cc-pV5Z, cc-pV6Z.

Keywords:

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2-Propanol

1-Propanol

H-ZSM-5 zeolite

Water

Propene

Catalysts