Abstract Submitted
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A Computational Study of Catalytic Dehydrogenation of Propane to Propene Using Transition Metal Atoms[1] MICHAL SCHERER-BERRY, CHRISTOPHER BEAN, DANIEL DUNEVANT, NICK LEWIS, STAN ZYGMUNT, Valparaiso University — Developing more reactive and selective catalysts for petrochemical refining and synthesis, specifically the dehydrogenation of propane to form propylene, is extremely important for the US and global economy. The use of single atom catalysts can potentially tune their catalytic properties for specific reactions. Using computational methods, the dehydrogenation reaction pathways of possible catalysts with propane can be tested; however, this can be very time consuming. By looking at possible simple descriptors of promising catalytic behavior, the time spent testing specific alloys can be greatly reduced. We have evaluated various descriptors and hope to find correlations between these and the more time-consuming factors in order to help discover which transition metal clusters can be used to lower the cost of propane dehydrogenation.

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