Reaction mechanism between Gen (n=2-5) clusters and single water molecule based on Density Functional Theory

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Abstract

Density functional theory (DFT) was used to calculate the most stable structures of Gen (n=2-5) clusters as well as the adsorption energies of Gen (n=2-5) clusters after adsorbing single water molecule. The calculation of the reaction paths between Gen (n=2-5) and single water molecule shows that water molecule can react with Gen (n=2-5) clusters to dissociate to produce hydrogen, and O atoms mix with the clusters to generate GenO (n=2-5). According to the energy change of the reactions, the Ge2 cluster is the most efficient among Gen (n=2-5) clusters reacting with single water molecule. The NPA and DOS respectively proved that the Ge atoms in the product don't reach the highest valence, and it was jointly predicted that GenO (n=2-5) might continue to react with more water molecules. Our findings contribute to better knowledge of Ge's chemical reactivity, which could aid in the development of effective Ge-based catalysts and hydrogen-production methods.

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