Reactivity of Aluminum Cluster Anions with Water: Origins of Reactivity and Mechanisms for H_2 Release.

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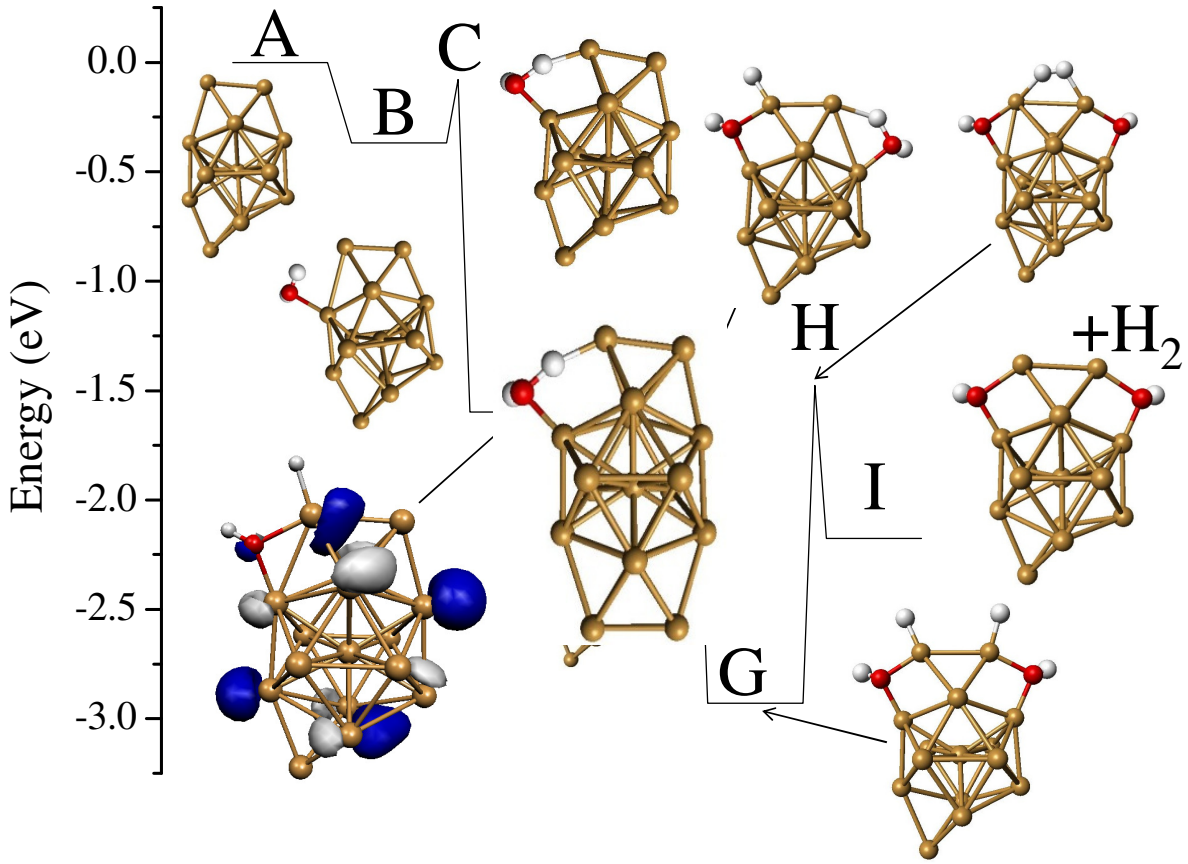

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gure S1. Reaction coordinate for the formation of H_2 from Al_{16}^- and $2H_2O$ molecules. A) is Al_{16}^-, B) is with an intact water molecule bound to the cluster, C) is the transition state for splitting the first water, D) is cluster after water is split, with the LUMO+4 charge density to show the induced Lewis acid site. E) is after the second water is bound, F) is the transition state for splitting the second water, G) is after the breaking of the second O-H bond, H) is the transition state for releasing H_2, and J) is the final cluster after H_2 is released.

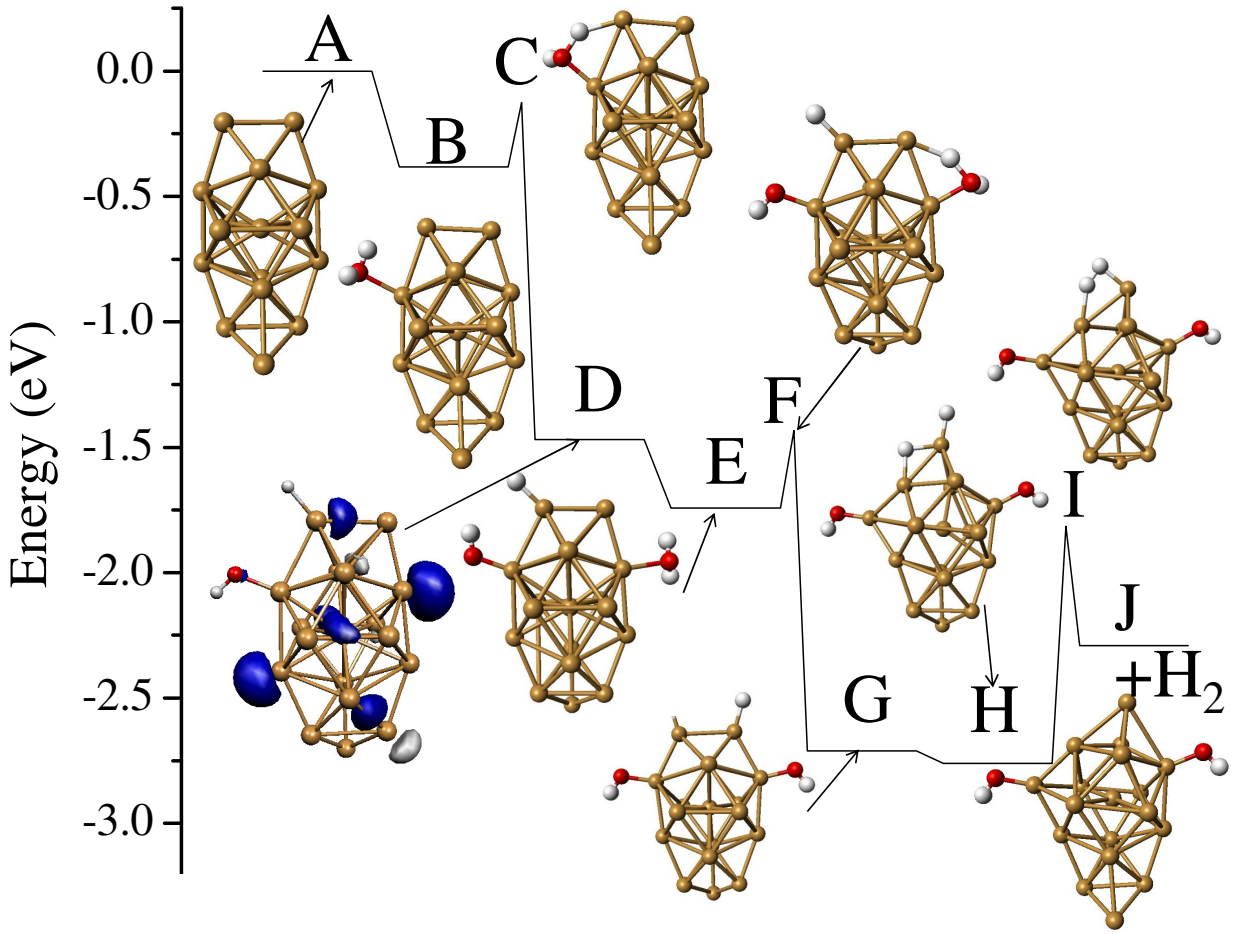

Figure S2. Reaction coordinate for the formation of H_2 from Al_{18}^- and $2H_2O$ molecules. A) is Al_{18}^-, B) is with an intact water molecule bound to the cluster, C) is the transition state for splitting the first water, D) is cluster after water is split, with the LUMO+4 charge density to show the induced Lewis acid site. E) is after the second water is bound, F) is the transition state for splitting the second water, G) is after the breaking of the second O-H bond, H) is a rearrangement of the cluster to facilitate the release of H_2, I is the transition state for releasing H_2, and J is the final cluster after H_2 is released.