

First-Principles Study of Stability and N₂ Activation on the Octahedron RuRh Clusters

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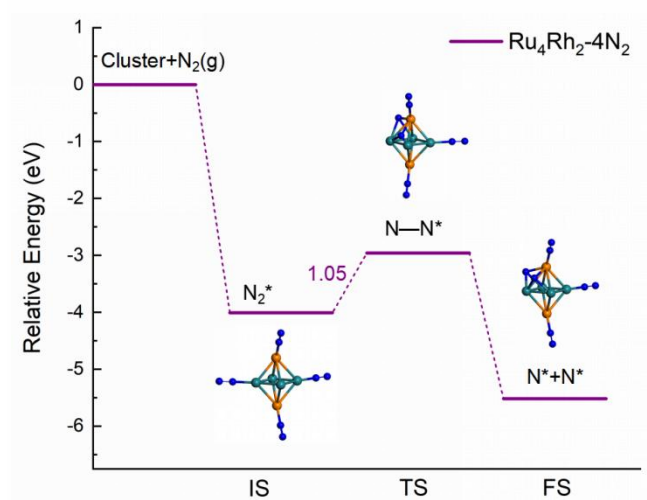


Figure S1. Potential energy surface comparing N₂ dissociation on Ru₄Rh₂ cluster. Geometric structure of the IS, TS, and FS of four N₂ molecule in elementary reactions on Ru₄Rh₂ cluster.