

Gold and Aluminum clusters as catalytic agents: Study of structure and reactivity using density functional theory

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Abstract: Metal clusters have been of importance as catalytic agents in recent years. We present in this talk our study of structure and reactivity of small clusters of gold and aluminum clusters and the relativistic effects, in particular, on the gold clusters. Our studies provide insight on the structure and reactive atoms in gold clusters as oxidation catalysts. High energy conformers of Aluminum clusters, on the other hand, are shown to be excellent candidates in activation of nitrogen molecule.