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Ab-initio study of gold nanoparticles supported on defect-laden single-layer MoS2[1] TAKAT B. RAWAL, DUY LE, TALAT S. RAHMAN, University of Central Florida — We have investigated the geometry, electronic structure, and catalytic properties of gold nanoparticles on defect-laden single-layer MoS_2 using density functional theory (DFT) based calculations with semi-empirical van der Waals interaction (DFT-D3). Our results show that the two-dimensional planar structure, the most favorable one for unsupported Au_{13} nanoparticle, transforms into a distorted three-dimensional (3D) structure when supported on single-layer MoS_2 with single S-vacancy which is more favorable than the icosahedral, decahedron and cuboctahedron forms. The MoS_2 support substantially alters the electronic structure of Au_{13} nanoparticle near the Fermi level, owing to the strong interaction of MoS_2 support with Au_{13} in the presence of an S-vacancy. The modified electronic structure remarkably affects the catalytic activity of the MoS_2-supported Au_{13}, offering enhanced activity towards methanol synthesis reaction via CO hydrogenation reaction - a contrast from that of titania-supported Au_{13} nanoparticle [1] which promotes methanol decomposition. [1] S. Hong and T. S. Rahman, JACS, 135, 7629 (2013)

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