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First principle study: adsorption of molecular hydrogen sulphide on transitional gold cluster (Aun=1-5)

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Abstract content
   (Max 300 words)
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We present theoretical results of the study of H2S adsorption on gold cluster Aun(n = 1- 5) using density functional theory with Perdew-Burke-Ernzerhof (PBE) exchange-correlation energy functional. Minimum energy structures of the gold cluster along with their isomers are considered in the optimization process. H2S molecule is observed to adsorb on to the gold cluster. However, the adsorption energy decreases with increasing cluster size. The structures of the gold clusters are similar before and after adsorption of H2S molecule. The structures of gold cluster remain planar. The adsorbed molecules get adjusted in a way that their center of mass lie on the plane of the gold cluster. The adsorbed molecules get attached to a single gold atom and there is no preference to get adsorbed in between the gold. H2S dissociation is not favoured on the Au clusters since it demands extra energy to dissociate which is costly.

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