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Theoretical analysis of molecular oxygen adsorption on the silver claster Ag_4

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Abstract

In the present work quantum-chemical calculations of adsorption interaction energies were carried out in the systems containing four-atom silver cluster as well as molecular adsorbed oxygen located at different adsorption sites with respect to the cluster surface. The calculations were performed at HF/DGDZVP and B3LYP/DGDZVP levels of theory. It was shown that the HF/DGDZVP level of theory allows obtaining a qualitative model correlating well with experimental data. However, this method does not provide an appropriate precision when describing adsorption interactions, while the B3LYP/DGDZVP provides an adequate accuracy. It was stated that molecular oxygen participates in oxidative catalytic processes, carried out over the silver-containing catalyst surface, in its singlet state.