INFLUENCE OF DFT-FUNCTIONAL AND BASIS SET OF FUNCTIONS ON CALCULATION RESULTS OF THE STRUCTURAL AND ENERGY PROPERTIES OF Ag2 MOLECULAR CLUSTER

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Abstract

The paper deals with the impact assessment for the exchange-correlation functionals and Slater-type basis sets on the properties of molecular cluster Ag2 carried out within the framework of the density functional theory. For comparative analysis of these properties equilibrium bond length and the total binding energy of the molecular cluster were used. The effect of the change of all-electron basis sets dimension within four exchange-correlation functionals of different categories was analyzed. We also discuss the results obtained for the basis sets with different levels of frozen-core approximation. Results obtained with the gradient corrected exchange-correlation functionals and all-electron QZ4P basis set show the best agreement with the experimentally determined values. Small size frozen-core approximation reduces the computation time, and the deviation of the calculated values of the binding energy takes a smaller value compared to all-electron basis sets. The results are of methodological interest for the correct calculation of the characteristics of molecular clusters with the expected accuracy.

Keywords: density functional theory, quantum chemical calculation, molecular cluster, silver, exchange-correlation functional.

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