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QUANTUM CHEMICAL MODELING OF ADSORPTION PROCESS AT FLOTATION ON THE CLUSTER OF SPHALERITE AND WURTZITE

Abstract. A quantum-chemical calculation of the behavior of molecule on the surface of sphalerite and wurtzite is carried out using the views of Density Functional Theory (DFT). Energy minima are determined from the geometric coordinates of the molecule corresponding to the ground and metastable states, clusters of sulfide minerals of sphalerite and wurtzite are constructed. An orbital analysis of the studying system has been carried out, and the orbitals have been restructured during the interaction of this system.

Key words: cluster, sulphide, minerals, sphalerite, wurtzite, Density Functional Theory molecular modeling.

The models of estimation the interaction of mineral-sulfides system using quantum-chemical methods have become widespread. The essence of such studies is that the very difficult problem of interaction with the surface of solid reduces to the calculation of simple models which reflect the basic properties of the complex. Well known, the two types of model approaches are most widely used: solid-body models which take into account the "collective" properties of solid, and molecular models that take into account only a part of the solid (cluster). At present time the latter method have been widely used in the quantum-chemical investigation processes. It should be noted that the role of molecular modeling in chemistry is quite large, despite the obvious priority of experimental research in this field of natural science. The most significant are theoretical results that are impossible, extremely difficult or too expensive to obtain by experimental means [1, 2]. Traditionally, modeling tasks include the definition of the structure of individual molecules, molecular associates or fragments of solids, as well as the description of the mechanisms of chemical reactions at the molecular level. Such modeling is most often in recent years carried out using the methods of quantum chemistry.

The attractiveness of molecular models to estimate the reactivity of minerals-sulfides with respect to a certain reagent consists in the possibility of taking into account the structural-geometric and chemical heterogeneity of the surface of solid. In this case, the establishment of correlation with the experimental data is great importance for evaluating the correctness of the calculations. The results of the experimental study are also very important, when choosing the initial model [1-3].