

Binding energy of a silicon adatom with the clusters modeling different positions on the amorphous silicon oxide surface

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Information on binding energy of a silicon adatom in different positions on the amorphous silicon oxide surface is necessary for molecular dynamics and Monte Carlo modeling of silicon nanoclusters nucleation and growth processes. The principal structure properties of such positions may be reflected to the first approximation with the use of simple silicon-oxygen clusters. Such clusters may be made so as a silicon adatom could create a required number of bonds with surface oxygen and silicon atoms. In the work different simple silicon-oxygen clusters were used for obtaining all possible hypothetical positions of a silicon adatom on the amorphous silicon oxide surface. A number of adatom bonds with surface oxygen and silicon atoms varied from one to four. Total energy calculations were performed with the density functional theory (DFT) approximation using the quantum chemistry Gaussian 98 code. The combined B3LYP functional and several basis sets up to 6-311++G(3df,3pd) were used. In the first place the geometry optimization and the calculations of total energy and own frequencies were performed for the initial cluster containing a silicon adatom. In the second place such calculations were performed for the cluster obtained from the initial one after tearing off an adatom. On the whole the results on influence of the number and type of bonds on the binding energy of a silicon adatom were obtained. The obtained results have allowed to reveal a number of tendencies peculiar to interaction nature of a silicon adatom and small clusters with the amorphous silicon oxide surface. On results of the work it is possible to do a number of suggestions with regard to possibility of the use of the cluster approach for the decision of the question on the interaction energetics of silicon adatoms and small clusters with the amorphous silicon oxides surface. In connection with essential influence of relaxation phenomena at tearing off silicon atoms that are connected with forming the new bonds, the values of binding energy obtained without taking into account relaxation phenomena have to be used as the comparative energetic characteristic. When considering concrete situations of interaction of a silicon adatom and small cluster with the necessary number of oxygen and silicon atoms it is advisable to use the cluster most large and greatly approaching to structure of the silicon oxide. The results obtained using the 6-31G(d) basis set can be considered as enough correct. The use of more powerful basis sets makes the results more precise but requires a considerable amount of time for the calculations of the most large examined clusters. It may be supposed that for complex situations of the interaction of silicon atoms and small clusters with the amorphous silicon oxide surface, for which the experimental and more exact calculation data are absent at present time, the results on binding energy obtained in the cluster approach can serve as the quite correct first approximation.

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