Changes of occupation of electronic levels of adatoms on the surface of solids at changes of the state of some active places of the surface.

A. Z. Shekhtman *
KVANT
Moscow, Russia

One of the main properties of active catalytic places on solid surface is their ability to make reacting species close to enhance possibility of their reaction. These places are a main component of a catalytic reaction. So it is interesting to study a catalytic reaction in the framework of an approach that allows us to simultaneously take into account all components of such reaction. Such approach is convenient also to study changes of the electronic structure of adatoms depending on competition of different contributions in their energy including contribution of the exchange interaction at very small distances between adatoms at changes of the state of some active places on the surface of solids.

Here, the results are presented that were obtained on the basis of one of such approaches. The work was done in the 1980-s in connection with a study of catalytic reactions on surfaces of solids. We considered interaction of two two-levels adatoms on the surface of a simple metal model with uniformly distributed atoms of the metal. The task was solved in the framework of approximation of the density functional. We took into account direct dipole-dipole interaction of the adatoms, exchange interaction, indirect interaction through conductivity electrons, and an effective attraction of the adatoms to some point of the surface (a relatively long-distance attractive factor). Depending on values of the selected parameter of the effective attraction of the adatoms, the solution of the set of the equations for the numbers of occupations of two electronic levels of two adatoms gave us different possible states of the considered system of adatoms. They were states with equal and unequal occupation of the levels, states that can be considered rather like a state of a set of two interacting separate adatoms or rather like a state of an adsorbed molecule and so on. It is interesting, that depending on values of the selected parameter, the state of the system showed either electronegative or electropositive character of adsorption.

Certainly, the considered problem is very simplified, but in the framework of the same approach we can study influence of some external conditions on the electronic structure of adatoms at more realistic assumptions.

Acknowledgements

The author would like to thank his eldest son for the support of the study.

References

***Current address: 71 Alicante Aisle, Irvine, CA 92614,USA.**