Construction of the adiabatic potential of a symmetric molecule in the vicinity of charged surface of semiconductor

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A correct solution of the problem connected with a construction of the adiabatic potential by means of group theory allows one to use the adiabatic potentials for a qualitative explanation of wide variety of physical phenomena related with vibronic coupling. In particular, these potentials are extremely useful for interpretations of IR-, Raman-, photo- and X-ray spectroscopy data, as well as in the theory of chemical reactions and catalysis.

In the work, we show a construction of the vibronic potential and the corresponding adiabatic potential for a molecule with D_{3d} symmetry by means of the group-theory methods supplied with the Pikus' method of invariants [1]. The symmetry of normal vibrations of a molecule which are active in Jahn-Teller effect [2] has been established. The vibronic coupling of the E–E type leading to obtain the vibronic potential energy in a matrix form and of the adiabatic potentials has been investigated earlier [3]. The application of adiabatic potentials can be important in the theory of phase transitions caused by the vibronic interaction (the so-called cooperative Jahn-Teller effect) and in issues of chemical catalysis and interaction of molecules with an atomic surface. It is known that a newly prepared surface of a material is charged. To eliminate the charge on this surface a passivation procedure is usually used. This procedure relies on a surface irradiation by the hydrogen ions. On the other hand, to clean a surface, resulting in it becoming charged, the flow of helium atoms is used. Charged surface exhibits an electrical field which is perpendicular to the surface. If a stream of molecules swoops to such a surface, a problem of theoretical study on the stability of the molecule in an electric field arises. In order to solve this problem, in this work we extend a procedure of the adiabatic potential construction which was presented in [3] for an isolated molecule. We demonstrate that the influence of an external field on a molecule near a charged surface can also be taken into account by the methods of the theory of symmetry. We find the polarization vector **p** components and of the quadrupole momentum tensor *Q* which are totally determined by the symmetry of the investigated molecule and by the direction of the electrical field. Taking into account the symmetry of the considered molecule, we obtain additional elements (with respect to those obtained in [3]) in the vibronic potential energy matrix and construct new terms of the adiabatic potential.

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