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AUTHOR: (10) Nagayev, E.L.

TITLE: (6) On the theory of chemisorption on polar crystals

PERIODICAL: (21) Kinetika i kataliz, v.3, no.6, 1962, 907-914

TEXT: The adsorptive properties of crystals are determined predominantly by the relative proportions of polar and homopolar bonds in crystals. For a perfectly polar crystal the adsorbed molecule gives up one of its electrons to the crystal with the resulting energy gain. For a purely homopolar crystal the adsorbed molecule retains its electrons and a three-electron bond results. An adsorbed atom forms a strong two-electron bond with homopolar crystals, but a weak single electron bond is formed with polar crystals. The strength of adsorption of an atom on a crystal is the greater the higher the proportion of two-electron bond. This proportion increases with the homopolar character of the crystal and its narrowing forbidden zone. The energy of dissociation of an adsorbed molecule decreases as the forbidden zone narrows. In the presence of certain defects on the surface the adsorption near the defects is favoured energetically. For Card 1/3

monovalent electro-positive atoms adsorbed near a relatively highly charged ion, replacing a weakly charged cation in the crystalline lattice, the energy of adsorption is higher than that on the ideal surface. Conversely the energy of adsorption of a molecule near the defect decreases and the activation energy increases compared with the energy of adsorption on the ideal surface. If the charge of an ionic impurity is smaller than that of the cation that the ion replaces, the activation energy of chemisorption near such a defect decreases and the bond strength between the adsorbed molecule and the surface increases, the bond strength for the adsorbed atom also decreases. The authors indicate that it would be desirable to check experimentally the postulated theories by 1) checking the dependence of the character of chemisorption on the width of the forbidden zone; this could be done by conducting experiments on pure surfaces at low temperatures, which should give low concentrations of the supports in the surfaces and 2) investigating the effect of surface defects in the surfaces with the concentration of the support small in comparison to that in the bulk of the crystal. Card 2/3

There are 4 figures.

ASSOCIATION: Nauchno-issledovatel'skiy institut  
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