Role of charge transfer at surfaces in determination of adsorption energy - consequences to vapor growth and doping of semiconductors

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The model is proposed indicating that charge transfer between surface and the bulk of semiconductor may affect the adsorption energy considerably. The process may change the adsorption energy, depending on the availability of empty states at the surface and pinning of Fermi level at the surface. In case of the nonpinned Fermi level, the adsorption energy depends on the doping in the bulk. The results of DFT calculations confirm these predictions. Adsorption of several molecular species, pertinent for crystal growth of the semiconductors at the polar surfaces of GaN, SiC and ZnO were investigated. The investigated cases include adsorption of ammonia and hydrogen at polar GaN(0001) surface, hydrogen, silicon and carbon at SiC(0001) surface and zinc and oxygen at ZnO(0001) surface. Crystal growth from the vapor is reviewed showing that the adsorption of growing species leads to the increase of the adsorbate to the point where Fermi level is unpinned. Thus majority of the growth processes occurs at this condition, so that the adsorption depends on the doping in the bulk. This mechanism explains the dependence of the growth and doping on the Fermi level in the bulk. These predictions are verified by thermodynamic analysis of the growth of GaN, SiC and ZnO with application of DFT data.