THE COVALENT-BAND MODEL OF HYDROGEN KEEPING IN FULLERENE AND OF THE CATALYSIS

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Semiconductor (s/c) state of fullerene (FUL) is broken by solution of H ions on its net. The theory must take into account not only the covalent C–H-bonds, but also the appearance of admixture conduction band (band electrons). The many-electron operator spinors (MEOS) representations for C- and H-ions and the Fermi operators of band quasi-particles (electrons and holes) define the Hamiltonians of their interactions. The basic part of covalent energy Γ^{C-H} predominates over the bond energy of H_2 molecule and breaks up it. H-ions either remain on FUL net, or penetrate into FUL volume. The equations of their states depend on H_2 kinetic energy. H concentration on FUL net depends on temperature T through the function $\Gamma^{C-H}(T)$. The activation energy of H diffusion on FUL is $E_a \sim \Gamma^{C-H}(T)$.

The chemical (covalent) bond fluctuations (CBF) are represented by the Fourier image of MEOS. They form the thermal part of covalent energies. The combinations of CBF spectra and ionization energy E_0 of C ions are parts of expressions for the width of forbidden band $E_g(T)$. They define mobilities of electrons and holes in s/c state and possibility of FUL metallization changed. (the Fermi energy ε_F), when H concentration is

CBF contribution decreases $\Gamma(T)$ and $E_a(T)$. This favours H-ions leaving FUL. H-ions diffusion on FUL net favours catalysis. The breaking up of N_2 and other molecules and their bond with FUL net are considered by analogy with H_2. The collision of diffusible (with different velocity) H and N ions favours the formation of H_4N and other molecules. The theory allows calculating the chemical reaction rate (with catalysis on FUL) at different temperatures [1].

The calculated dependence of H concentration within FUL on temperature allows calculating H absorption, its keeping in FUL system and its extraction from this system at heating, the influence of magnetic field (taking into account magnetic state and magnetic admixture in FUL [2]), pressure, etc.

References

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