## Nanochemistry and Nanobiotechnology

# Energy of interfacial reactions in the processes of mechanical separation of hematite and silica nanoparticles

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Flotation technology is nanotechnology on the physics and chemistry processes occurring at the interface of the liquid, solid and gaseous phases at distances measured in tens of angstroms [1]. Flotation is not only determined by the mechanical attachment of the solid particles to the gas-liquid interface, but the adsorption processes and the heterogeneous chemical reactions determine it. The most complete treatment of these processes requires an analysis of the total energy of these systems and distribution of electron density on interface. Look at the interface of solid-liquid-gas interface at the atomic scale is possible only with the help of the first-principles quantum chemical calculations (electron density functional theory).

This paper analyzes the flotation processes applied oxidized iron ores of the Kryvyi Rih basin: a mixture of hematite ($\alpha$-$Fe_2O_3$) and quartz (CaO), water bathed with additional organic reagents. The structure of hematite is the same as ($\alpha$-Al2O3), the corundum structure, which is based on a hexagonal close-packed anion packing. The unit cell is hexagonal, with a= b=5.04 Å and c=13.75Å. The Fe-terminated {0001} surface is the natural plane of hematite and has lower surface energy than the oxygen-terminated and all other surfaces of hematite. We have studied the electronic structure of the (0001) hematite ((100) quartz) surface using *ab initio* methods to interpret experimentally data [2], but also to gain insight into atomic level changes in electronic structure that are associated with heterogeneous surface reactions. All calculations have been made with the proprietary source code [2]. A number of eight valence electrons for each Fe atom ($3d^7 4s^1$) and six valence electrons for each O atom ($2p^2 2p^4$) were taken into account. The core electrons together with nuclei were described by *ab initio* BHS pseudopotentials, the exchange-correlation interactions were described by local density application. Changes of electronic potential at the interface of hematite and quartz in water and solutions of reagents were obtained.

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2. *Balabai R.M.* Electronic properties of functionalized graphene nanoribbons // Ukr. J. Phys.- 2013.-**58**, N 4.- P.389-397.