KINTECH LABORATORY

From atoms and molecules - to new materials and technologies

Program "NANO"

Background

The program "NANO" is designed to determine the density distributions of conduction electrons ($n_c(\boldsymbol{r})$) and positively charged ions ($n^+(\boldsymbol{r})$) inside a semiconductor nanoparticle. It provides the solution of the problem using newly developed method and as a result gives the extreme distribution functions for $\boldsymbol{n}_c(\boldsymbol{r})$ and $n^+(\boldsymbol{r})$, as well as N_c and N_O-. The potential corresponding to the minimum of the nanoparticle free energy could also be obtained. This program of searching for extreme charge distributions in nanoparticles proves to be invaluable in solving problems associated with various physicochemical and electrophysical properties of nanomaterials. Such properties include conductive, sensory, photoelectric, catalytic, magnetic, dielectric, and plasmon properties. The importance of this program for solving various problems of nanobiophotonic should also be noted.

Solution method

The program "NANO" is included in the package **Chemical Workbench®** This program is designed to determine the density distributions of conduction electrons ($n_c(\boldsymbol{r})$) and positively charged ions ($n^+(\boldsymbol{r})$) inside a semiconductor nanoparticle, as well as the number of charged electron traps on the surface (N_O-). These parameters are determined from the condition of minimum free energy of nanoparticles. The free energy F represents the sum of four terms ($F = F_1 + F_2 + F_3 + F_4$), where F_1 is free energy of conduction electrons, F_2 is free energy of donors, F_3 is electrostatic energy, and F_4 is free energy of surface traps. In addition, the distribution functions $n_c(\boldsymbol{r})$ and $n^+(\boldsymbol{r})$ satisfy the normalization conditions, which include the values of N_O- and N_c, the number of conductive electrons.

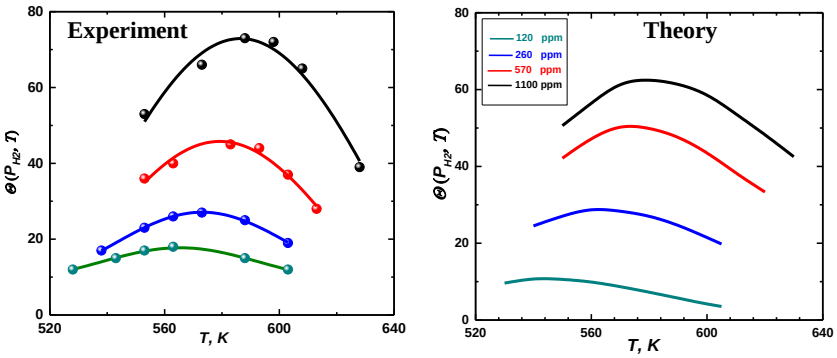
An original method of solving this problem is developed. The method essentially reduces to multiple solution of boundary value problems for a system of differential equations (the Euler system), which results from the variation of the functional F. Because of the complicated form of the functional F, fulfilling its variation is a nontrivial task. In solving boundary value problems for the Euler system, the relaxation method with an implicit finite-difference scheme is applied. The essence of the method is that the time derivatives of unknown function are added to the stationary equations. Therefore, it is necessary to solve the auxiliary non-stationary problem instead of a stationary one. The solutions of non-stationary and stationary equations obviously approach each other when the time tends to infinity. The non-stationary problem exists until its solution ceases to vary within the required precision level.

Note that for the calculation of the values of the functional, it is necessary to know the value of N_O, which is the total number of surface traps. The value of N_O depends on the process under consideration. In particular, such a problem was solved for the conductivity and sensory process. An algorithm is proposed for the solution of the resulting system of equations for stationary concentrations of positive charges and electrons at both inside the nanoparticle and the surface. The electrons captured by oxygen atoms on the surface also are taken into account. The reactions of O^- with surrounding molecules could also be readily considered.

Comparison to experiment: In_2O_3 sensor response at hydrogen detection

Black – 1100 ppm
red – 570 ppm
blue – 260 ppm
green – 120 ppm

M.A. Kozhushner, V.L. Bodneva, I.I. Oleynik, T.V. Belysheva, M.I. Ikim, L.I. Trakhtenberg, ***Sensor Effect in Oxide Films with a Large Concentration of Conduction Electrons*** // **J. Phys. Chem. C. 2017**. V. 121. P. 6940-6945.



The algorythm was developed by: **V.S. Posvyanskii, B.V. Lidskii, V.L. Bodneva, M.A. Kozhushner, L.I. Trakhtenberg**

Contacts
Kintech Lab, Ltd.,
1, Kurchatov Sq., Moscow,
123182, Russian Federation

☎+7 (499) 704-25-81
🖷 +7 (499) 704-25-81
info@kintechlab.com
www.kintechlab.com