ODD ELECTRONS IN NANOMATERIAL SCIENCE. A NEW APPROACH TO COMPUTATIONAL CHEMICAL ENGINEERING

E.F.Sheka

Research Department, Peoples` Friendship University of the Russian Federation, Moscow

E.F.Sheka
Research Department, Peoples` Friendship University of the Russian Federation, Moscow

One cannot but share the concern expressed in the society over how hazardous are nanomaterials and how reliable are (if any) precautions which are or should be undertaken meeting their entering the living world (see Prof. R.Clift, *Nanotechinsight*, 1, Sept.2006). One cannot but agree with Prof. Clift as well that so far there has been no both toxicological and epidemiological evidence of the concern but that the conclusive and convincing testing will not appear in the near future due to enormously high price of *in vivo* and *in vitro* tests, both in time and cost. On this ground, *in silico* testing via computer modeling seems more feasible and promising. Suggested Quantitative-Structure-Activity-Relationship (QSAR) approach may accumulate size, shape and surface conditions that classify nanomaterials and show the way of the prediction of their behavior. There is a time for the QSAR approach to start since a great number of data in the field of computational nanatechnology obtained by now makes possible to generalize them towards establishing relationships.

The paper presents first results on the way concerning a peculiar aspect of nanomaterial science caused by *odd electrons*. The term stands from the difference between the number of atom valence electrons and that one of the neighboring atoms coupled to the considered one. The situation is so frequently met for nanomaterials that odd electrons should be added to size, shape, and surface conditions as one of the main characteristics of nanomaterials. Actually, chemical susceptibility of fullerenes and carbon nanotubes, peculiar characteristics of covalent nanocrystallite surfaces, and nanomagnetism seem absolutely different at first glance while being of the same origin. Basing on the feature, one can suggest a unified theoretical and/or computational approach to all the phenomena making possible their consideration on the same conceptual basis as well as on the same computational footing.

Peculiarities of nano-sized systems behavior directly depend on the odd electron coupling. Thus, in the case of benzene molecules, those are strongly coupled and fully covalently bonded, so that the species does not show any peculiar (radical) properties. Oppositely, in fullerenes [1] and carbon nanotubes [2] the coupling is weak so that they behave completely different. The bare silicon surfaces are magnetic [3-6] while the same carbon surfaces are not. Difference in the magnetic properties of the bulk traditional magnetic solids and their surfaces as well as nanoparticles, different magnetic behavior of solids composed of molecular nanocomplexes of the same structure but differed by transition metals atoms (say, Ni and Co) etc. follow from the difference in coupling of the available odd electrons as well.

The quantum theory of the electron bonding is suggested as the computational basis for the events. One-determinant Hartree-Fock approach has been shown [7] to provide a correct quantitative determination of both *chemical* and *magnetic susceptibilities* of odd electrons that lays the foundation of a generalized odd-electron QSAR, which covers a large class of nanomaterials, to be obtained.

Literature

1. E.F.Sheka: Int.Journ.Quant.Chem. 100 (2004) 375.
2. E.F.Sheka, L.A.Chernozatonski. J.Phys.Chem. A (submitted).
3. V.Khavryutchenko, E.Sheka, D.-H.Huang, M.Aono. Phys. Low-Dim. Struct., No 3/4 (1998) 81-106.
4. E.F. Sheka, E. A.Nikitina, V. A.Zayatz. Surf.Sci. 532-535 (2003) 754.
5. Z.Wu, T.Nakayama, M.Sakurai, M.Aono. 2000. First International Symposium on Nanoarchitechtonics Using Suprainteraction – NASI-1 (Tsukuba, Japan, 13-15 November 2000).
6. V.Venkataraman, K.Nogushi, M.Aono, T.Suzuki. Appl. Phys. B 74 (2002) 683.
7. E.F.Sheka, V.A.Zayets. Russ Journ.Phys.Chem. 2005**,** 79 (12), 2009.