Nanocomposites and nanomaterials

Impossible is nothing: Using unified description methods for bulk and nano materials

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In more than 50 years of active development, the field of quantitative structure-activity relationships (QSAR) modeling has grown tremendously with respect to the diversity of both methodologies and applications [1]. Researchers solved a lot of different tasks starting from prediction of solubility of phenolic compounds and finishing with nanoparticles characterization.

To make QSAR theoretical modeling, each particle should be described by numerical parameter, called descriptor. Chemical descriptors are at the core of QSAR modeling, and so many different types of chemical descriptors reflecting various levels of chemical structure representation have been proposed so far [1].

Unfortunately, modeling of nanoparticles is challenging because of the high complexity. They consist of great number of individual molecules and properties of nanoparticles dramatically differ from analogous properties of individual molecules. It is clear, that traditional QSAR approaches seem to be much more problematic than in case of “classical” chemicals.

In the current study it was shown that developed in-house Simplex Representation of Molecular Structure (SiRMS-based descriptors) [2] and “Liquid Drop” model (LDM-based descriptors) [3] are useful for QSAR investigation of different properties of different types of materials from bulk to nano-sized materials.

In addition, another studies presenting nano-QSAR models were analysed. Special nano-oriented descriptors and regular methods of structural representation were compare.

1. *Cherkasov A. et al.* QSAR Modeling: Where Have You Been? Where Are You Going To? // J of Med Chem. Article ASAP.
2. *Kuz’min V.E. et al.* Virtual screening and molecular design based on hierarchical QSAR technology. // Challenges and Advances in Computational Chemistry and Physics. – 2010. – **8**. – p. 127-176..
3. *Smirnov B.M.* Processes involving clusters and small particles in a buffer gas // Phys. Usp.-2011.-**54.**-P. 691–721.