Chapter 49
Nanoparticles: Towards Predicting Their Toxicity and Physico-Chemical Properties

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ABSTRACT

Nanomaterials are becoming an important component of the modern life and have been the subject of increasing number of investigations involving various areas of natural sciences and technology. However, theoretical modeling of physicochemical and biological activity of these species is still very scarce. The prediction of the properties and activities of 'classical' substances via correlating with molecular descriptors is a well known procedure, i.e. QSAR. In spite of this, the application of QSAR for the nanomaterials is a very complicated task, because of "non-classical" structure of nanomaterials.

Here, the authors show that an application of the QSAR methods for nanomaterials is nevertheless possible and can be useful in predicting their various properties and activities (toxicity). In the chapter briefly explained how the physico-chemical properties can be predicted for nanomaterials. Furthermore, it was also demonstrated how the biological activity, particularly toxicity, can be modeled and predicted for the series of nanoparticles, by applying the quantum-chemical methods in combination with the nano-QSAR.

INTRODUCTION

During the last three decades there has been a dramatic increase of attention directed towards chemistry and technology of nanoparticles. The search by Google word search engine through publications for the period 1800-2008 indicates an enormous rise in frequency of the use of words "nano" and "nanoparticle" starting from 1980s. So, what is a nanoparticle? Nanoparticles are building blocks for nanotechnology, and are defined as particles (structures) with at least one dimension of less than 100 nm (Buzea et al, 2007). In fact, particles in these size ranges have been used by

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humankind for thousands of years. However, there has been a recent renaissance in this area because of the technological progress and therefore an ability to synthesize and manipulate such materials (Rotello, 2004). Nanomaterials are being currently used as electronics, optoelectronics, in biomedical, environmental, material and energy related areas, as cosmetics, pharmaceuticals, and catalysts. Nanomaterials exhibit unique physical/chemical properties and impart enhancements to engineered materials, including better magnetic properties, improved electrical activity, and increased optical properties. Because of the potential output of this technology, a worldwide increase in applications and investment in nanotechnology research are on rise (Srivastava et al, 2001; Klabunde, 2001; Feldheim, 2001; Edelstein & Cammarata, 1998). Moreover, the use of nanomaterials in various industries is projected to increase dramatically in the future and as a consequence, contamination of environment by these materials is expected, or at least such possibility cannot be disregarded. In fact, nanotechnology could lead to serious environmental problems. This is because it is still largely unknown how nanoparticles will impact the environment. Besides, there is still a substantial need to comprehensively investigate all physicochemical and then biological properties of nanoparticles to predict their possible impact on environment (Pitkethly, 2004; Oberdörster et al, 2005).

There is a clear need for short-term testing of their potential hazard in order to gain information towards risk assessment related to nanoparticles (Seatona & Donaldson, 2005; Seaton, 2007; Warheit et al, 2007). However, the large number of nanoparticles and the variety of their characteristics including sizes and coatings indicates that the only rational approach that avoids testing every single nanoparticle is to find relationship between physicochemical characteristics of a nanoparticle and its toxicity. For this purpose such approaches as Quantitative Structure-Activity Relationship (QSAR) can be applied (Puzyn et al, 2010; Puzyn et al, 2009). So, this approach can be applied not only to "classical" organic compounds (Kušić et al, 2009; Rasulev et al, 2007; Rasulev et al, 2010; Turabekova et al, 2008), but also for nanoparticles. If a QSAR model is developed then, ideally, toxicity of untested nanoparticle can be predicted on the basis of its physico-chemistry. Actually, there is a strong need to extend the traditional QSAR paradigm to nanoparticles, and some results related to this direction will be shown here.

Unfortunately, up to date, there is very limited information about systematic data on experimentally measured toxic effects for various series of nanoparticles. Only such data can be useful for the QSAR modeling purposes. However, some isolated and limited experiments are published in the last few years (Choi et al, 2008; Lewinski et al, 2008; Franklin et al, 2007; Duffin et al, 2007; Fiorito, 2007; Gill et al, 2007;Powers et al, 2007; Medina et al, 2007; Moore, 2006; Karakoti et al, 2006; Moss & Wong, 2006; Lee & Cho, 2006; Tsuji et al, 2006; Braydich-Stolle et al, 2005; Hussain et al, 2005). The available toxicity data for nanoparticles at this time are mostly *in vitro*, for bacteria cultures (Lewinski, Colvin & Drezek, 2008; Franklin et al, 2007; Duffin et al, 2007; Moss & Wong, 2006; Braydich-Stolle et al, 2005; Hussain et al, 2005). A few studies *in vivo* were published for mammals, particularly for rats or mice (Duffin et al, 2007; Gill et al, 2007; Medina et al, 2007). This limited toxicity information makes difficult the study of structure-toxicity relationship of nanoparticles.

In this chapter we have collected recent results related to our systematical investigations on QSPRs and QSARs of physico-chemical and toxicity endpoints for various kinds of nanoparticles. All these properties were studied by applying different computational approaches, including molecular modeling, and various quantum-mechanical calculations.