Chapter 51

QSAR–Based Studies of Nanomaterials in the Environment

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ABSTRACT

Nanotechnology is a newly emerging field, posing substantial impacts on society, economy, and the environment. In recent years, the development of nanotechnology has led to the design and large-scale production of many new materials and devices with a vast range of applications. However, along with the benefits, the use of nanomaterials raises many questions and generates concerns due to the possible health-risks and environmental impacts. This chapter provides an overview of the Quantitative Structure-Activity Relationships (QSAR) studies performed so far towards predicting nanoparticles' environmental toxicity. Recent progresses on the application of these modeling studies are additionally pointed out. Special emphasis is given to the setup of a QSAR perturbation-based model for the assessment of ecotoxic effects of nanoparticles in diverse conditions. Finally, ongoing challenges that may lead to new and exciting directions for QSAR modeling are discussed.

INTRODUCTION

The 21th century has witnessed a fast-dynamic growth of the nanotechnology field, leading in turn to the development of an innumerable number of nanomaterials with unique properties and a variety of applications in many sectors. However, the large-scale production and increasingly likelihood exposure to novel nanomaterials has spurred great concern regarding their potential adverse effects to humans and the environment. This chapter will provide an overview of *in silico* approaches developed so far for the prediction of nanomaterials environmental toxicity; from the use of classical approaches forward-

establishing Quantitative Structure−Activity Relationships (QSAR) to the applications of more evolved computational models. Particular attention will be paid to the setup of a new *in silico* perturbation-based model aimed at reliable predicting the ecotoxicity of metal-based nanoparticles under a wide range of experimental conditions.

NANOMATERIALS AND ENVIRONMENTAL RISKS

The idea that launched the new field nanotechnology started with the famous lecture "There's plenty of room at the bottom" given by physicist Richard Feynman at the Annual Meeting of the American Physical Society in 1959 (Feynman, 1960). In that meeting, Feynman wondered: "What would the properties of materials be if we could really arrange the atoms the way we want them?", foreseeing the production of materials at the nanometer scale with promising technical, industrial and biological applications. But the term "nanotechnology" was only coined decades later, firstly by Norio Taniguchi in 1974 within his inspections of ultra-precision machining (Taniguchi, 1974), and then by K. Eric Drexler in his 1986 book *Engines of Creation: The Coming Era of Nanotechnology* (Drexler, 1992). Though the real burst of nanotechnology didn't come until the early 1990s, with the development of sophisticated techniques for the characterization and manipulation of individual atoms such as scanning probe microscopy.

Nanomaterials are usually considered to entail materials that have single units with at least one dimension between 1 nm and 100 nm (Oberdörster et al., 2007). Nanomaterials can additionally be classified as one-dimensional (1-D), two-dimensional (2-D) and three-dimensional (3-D), according to the number of dimensions that are confined to the nanoscale range (< 100 nm). 1-D materials include nanofilms, nanolayers, and nanocoatings, while 2-D include nanotubes, nanorods, and nanowires. Finally, the most common 3-D materials are nanoparticles (NPs), the building blocks for nanotechnology applications. Nanomaterials can be amorphous or crystalline, be composed of single or multi-chemical elements, and exhibit various shapes and forms.

The advances in nanotechnology have made possible the development of many new materials and devices with a vast range of applications in medicine, cosmetics, electronics, biomaterials and energy production. Indeed due to the rapid pace at which nanotechnology is evolving and expanding into society via its applications, it is expected that many new innovative products containing manufactured nanomaterials will continue to vastly grow. Commonly, manufactured nanomaterials fall generally into two categories: carbon-based and metal-based materials (Bréchignac et al., 2007). Regarding carbon-based nanomaterials, these usually involve diamond, carbon-nanotubes, graphene and fullerenes, the latter being a class of allotropes of carbon that conceptually are graphene sheets rolled into tubes or spheres. Most of these nanomaterials are of interest for their mechanical strength and electrical properties (De Volder et al., 2013). Moreover, fullerenes in general are under study for potential medical applications, ranging from specific binding of antibiotics on resistant bacteria to even target certain types of cancer cells such as melanoma (Bakry et al., 2007; Simon et al., 2007). Carbon nanotubes for instance, have already been used as drug, gene, or protein carriers (Bianco et al., 2005). Nanoscale materials are being further developed in therapeutic modalities for advanced selective drug delivery systems and targeted nanotherapy (Ravi Kumar, 2000). Many of these modalities include polymeric NPs (Stupp et al., 2005), micelles (Kim et al., 2005), liposomes and dendrimers (Popat et al., 2007; Portney & Ozkan, 2006), hydrogels (Vinogradov et al., 2002), nanoshells (Zahr et al., 2005), and smart surfaces. The key performance characteristics of these materials are the high loading capacity, release kinetics, circulation time,

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