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Inexpensive and accurate - Novel computational methods for prediction of toxicity of nanomaterials

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Today, nanoparticles (NPs) have a wide range of applications in different aspects of human life. However, due to unique properties of NPs they could be harmful to the environment and humans. Therefore, it is a crucial role of scientists to uncover potential side effects of nanoparticles, inform the public, and provide solutions to the possible problems. There are various experimental techniques that are used to study different properties of nanomaterials, including their toxicity. However, such techniques are expensive to use and time consuming. There is a necessity to develop alternative methods, easy to use, fast, and efficient. Computational chemistry provides diverse tools that could evaluate molecular interactions among various species including nanoparticles and models of different biological species, and predict their properties and biological activities. The talk will be devoted to discussion of new challenges that nanomaterials create for the society. A part of the lecture will cover development of novel computational approaches, appropriate for evaluation of properties and activities of nanostructures. Current status of Nano-QSAR models will be discussed. The obtained results could be used as a first step in developing mechanisms that explain complex interactions of nanomaterials with biomolecules.

Biography

Jerzy Leszczynski, Professor of Chemistry and President's Distinguished Fellow at the Jackson State University directs Interdisciplinary Nanotoxicity NSF CREST Center. He has published about 800 referred papers and over 60 book chapters. He is editor of a book series: "*Computational Chemistry: Reviews of Current Trends*" (World Scientific;) editor of a book series *"Challenges and Advances in Computational Chemistry and Physics,"* (Springer); Editor of "*Handbook of Computational Chemistry"*(Springer); editor of book series "*Practical Aspects of Computational Chemistry"* (Springer), and "*Lecture Notes in Chemistry*" (Springer), and editor and member of editorial boards of eight journals.

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