Computational Approach to Nanomaterials by Design: From Quantum Chemistry to Artificial Intelligence

Anatoli Korkin

Adjunct Faculty, School of Molecular Sciences, Arizona State University, president of Nano and Giga Solutions, Inc.

Nowadays there is hardly any branch of materials science, from minerals to drug design, where computational approaches have not been used in combination with experimental techniques to develop new technologies and new materials with desired properties. Courses on computational materials tools are being introduced in major universities in all industrial countries at chemistry, physics, biology and engineering departments as complimentary or even as major expertise in research and engineering. Variety of computational techniques and their applications covers all type of materials and scales from small molecules (highly accurate *ab initio* quantum chemical calculations) to clusters made of hundreds and thousands of atoms (density functional theory - DFT) to (bio)polymers and amorphous materials (classical molecular mechanics and dynamics). Growing computational power and development of the new theoretical approaches gradually expend the areas of applications and predictive power of computational techniques. Chemoinformatics (or cheminformatics) has been introduced as a term in 1998 as branch of chemistry and informatics focused on analysis of various chemical data and molecular structure and topology for prediction of the chemical properties and reactivity. Nature inspired methods such as genetic/evolutionary algorithms and artificial neural networks have been developed and applied for materials science applications in combination with DFT calculations and data bases for materials structure and properties prediction. In my presentation I will provide an overview of various computational techniques and examples of their applications in different areas of materials science.