High-throughput materials discovery and development: breakthroughs and challenges in the mapping of the materials genome.

Marco Buongiorno Nardelli

Department of Physics and Department of Chemistry, University of North Texas

High-Throughput Quantum-Mechanics computation of materials properties by ab initio methods has become the foundation of an effective approach to materials design, discovery and characterization. This data driven approach to materials science currently presents the most promising path to the development of advanced technological materials that could solve or mitigate important social and economic challenges of the 21st century. In particular, the rapid proliferation of computational data on materials properties presents the possibility to complement and extend materials property databases where the experimental data is lacking and difficult to obtain.

Enhanced repositories such as AFLOW open novel opportunities for structure discovery and optimization, including uncovering of unsuspected compounds, metastable structures and correlations between various properties. The practical realization of these opportunities depends almost exclusively on the the design of efficient algorithms for electronic structure simulations of realistic material systems beyond the limitations of the current standard theories. In this talk, I will review recent progress in theoretical and computational tools, and in particular, discuss the development and validation of novel functionals within Density Functional Theory and of local basis representations for effective ab-initio tight-binding schemes.