Physics-Based and Data-Driven Multiscale Modeling of Nano-Materials

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Nanomaterials such as nanotubes, 2D materials, nanocrystalline materials, and nanocomposites, often have exceptional mechanical, optical, electronic, and thermal properties, thus show huge promise for a wide range of applications. Driven by advancements in experimental technologies and rise in computational power, a vast amount of data is being produced on nano-materials. In parallel, data-driven modeling has become an integral tool for scientific discovery of nano-materials for various applications, such as nanoelectromechanical devices, electronics and optical materials, sensors, surface coatings, energy storage, etc. However, depending solely on machine learning and ignoring the fundamental laws of physics may result in biased and non-physical solutions. A holistic modeling framework calls for the use of an ensemble of machine learning and physics-based modeling across the length and time scales of associated mechanisms for the nano-materials. Recent progress on integrating the machine learning and multiscale modeling shows promise in incorporating the underlying physics to enhance machine learning that yields to robust and efficient predictive models. The goal of this symposium is to understand the challenges and identify potential solutions for integrating machine learning and multiscale modeling applied to nano-materials. This symposium will solicit research presentations describing novel approaches in machine learning and multi-scale modeling for nano-materials providing deeper understanding on the interplay between physics, chemistry, engineering, and materials science. The symposium welcome contributions on machine learning and multiscale modeling applied to nano-materials. The topics of this symposium will include (but not limited to) the following: (1) Multi-scale modeling for mechanics and physics of nano-materials that may build upon ab-initio, molecular dynamics, monte carlo, or mesoscale modeling; Phase Field modeling of nano-materials; Modeling complex electro-chemo-mechanical processes influenced by thermodynamics, kinetics. (2) Data analytics for designing nano-materials for various applications including electronic, photovoltaics, fuel cells, thermos-electrics, 2D heterostructures; Metaheuristic optimization of material compositions and atomic structures; (3) Modeling for electronic, thermal and optical properties of nano-materials; role of defects and deformations; effect of edge energy, edge force, interaction of nano-materials with different substrates. (4) Machine learning for materials discovery – usage of recent developments in the fields of data mining, machine learning, and artificial intelligence for the identification of structure-composition-property relationships in the high diverse and sparse materials database. (5) Advances in the integration of machine learning and multi-scale modeling of nano-materials, such as accelerating molecular dynamics or ab-initio simulation using machine learning.