

Special Issue on  
**Predictive Models and Machine Learning Approach for  
New Nanomaterial Discovery**

# CALL FOR PAPERS

There is an ever-increasing need for developing new materials with novel electronic functionalities in the technology-driven modern society. To this end, a recent focus has been to integrate computational and experimental techniques for the purpose of obtaining robust, predictive tools for gaining insights into structure property relationships in functional nanomaterials in order to reduce time and cost in the materials discovery process. While a 1-to-1 approach (one system-one calculation-one experiment) has been the traditional strategy in nanomaterials research, this approach is quite inefficient due to the large experimental cost for preparing samples and for safe handling to avoid potential toxicity. Also without any predictive capability, the exploration for new functional nanodevice depends primarily on serendipity. To address many of these challenges and to cope with the increasing demands for novel functional nanomaterials, there have been worldwide efforts on developing new predictive strategies based on computational methods, machine learning tools, and materials information theory.

This special issue is intended to focus on compiling and updating the current status on the various predictive efforts based on informatics and computational methods and reviews on how successfully these new methods have addressed the grand challenges for designing and synthesizing novel nanomaterials in the laboratory. In connection with the newly developed popular material databases, the journal will also welcome reporting on major breakthroughs in nanomaterials research. Last but not least, the journal will provide essential information for the nanomaterials experimental community on how to leverage on these new predictive tools towards accelerated discovery of functional nanomaterials with emergent properties.

Potential topics include but are not limited to the following:

- ▶ Prediction and synthesis of stable and functional interfaces and heterostructures in nanoscale (semiconductors, VdW systems, etc.)
- ▶ Machine learning and nanoinformatics for nanoparticles with application in nanomedicine
- ▶ Synthesizing nanostructured materials with novel thermal, magnetic, optical, and electronic properties guided by computation and (or) informatics methods
- ▶ Computational prediction and experimental realization of functional nanomaterials with high structural stability, energy efficiency, and sustainability
- ▶ Nanoparticles in liquids and solids and discovering intercalating nanoparticles for enhancing functionality in bulk and layered materials
- ▶ The contribution and impacts of newly developed material databases and data mining tools on the experimental discovery of nanomaterials

Authors can submit their manuscripts through the Manuscript Tracking System at <https://mts.hindawi.com/submit/journals/jnm/pmmnn/>.

Papers are published upon acceptance, regardless of the Special Issue publication date.

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