



Foreword

Starting the pathway of *Materials Discovery*

This inaugural issue of the *Materials Discovery Journal* (MDJ) brings together a set of papers that represent the full scale of diversity in the modalities of materials science and engineering research; ranging from computational to experimental work; from inorganic to biological materials systems and from perspectives at the atomistic and molecular scales behavior to macro-scale engineering performance. Along with this cross-cutting taxonomy of contributions, all the papers address some aspect of data analytics and information science in a novel and unique way. These papers also capture the range in the genres of manuscripts MDJ is seeking to publish, from critical reviews to papers presenting new advances in original research.

Large and/or diverse data sets can be generated computationally or experimentally and both these topics are addressed in this inaugural issue. **McGinn** provides an incisive assessment of how to explore the complexity of coupling the generation of combinatorial libraries with the screening of properties in the complex realm of electrochemistry. **Takeda et al.** tackle a challenging problem in materials discovery based on combinatorial experimental studies, namely the interplay between materials chemistry and the form of the material (i.e. a powder or a single crystal) and their collective influence on properties. These authors describe a unique way to acquire high throughput data for single particle diagnosis in combinatorial experiments. Using microstructural simulation as a foundation, **Wodo et al.** present a unique computational framework for advancing the role of automation in data analysis. Using the template of microstructure-property relationships these authors address a challenging and often overlooked problem in materials databases systems, namely the importance of robust high throughput correlation analysis and not just searching for specific type of data. The value of such correlative analysis and data fusion, to materials characterization is demonstrated by **Boddupalli and Bratlie** in their work on multimodal imaging of collagen. The biological theme is expanded into the realm of nanostructures in the paper by **Packwood**, who shows how the use of appropriate statistical sampling techniques coupled to

simulations, can provide critical insight into mechanisms of peptide binding. Packwood's paper is also noteworthy as it takes advantage of the Open Data Pilot which the MDJ participates in which permits authors to contribute data and codes through a repository. The linking of atomistic scale simulation to a systems level impact of materials is demonstrated by **Golkaram and van Duin** in their application of reactive molecular dynamics to the study of materials toxicity. Finally, the theme of informatics from the perspective of data management, curation and standards is explored by **Austin** in the context of engineering properties who provides a timely review of the needs for establishing a digital infrastructure for materials design.

These inaugural papers provide evidence of the breadth and depth of analysis of the papers the MDJ is seeking from the community. MDJ strives to promote the concept of "materials discovery" utilizing all aspects of the emerging field of Materials Informatics including the understanding of the nature of data collection, interpretation of data, and advancing the understanding of the mechanisms governing materials behavior underlying the design and discovery of new materials.

The MDJ is fortunate to have a global community of distinguished advisors on the editorial board to help guide the growth of this new journal. Readers are encouraged to contact them or myself to propose topics for thematic issues for publication. Finally I want to thank the staff at Elsevier especially Dr. Baptiste Gault for all his support and help in guiding the establishment of MDJ and Sravanthi Sridharan, Journal Manager based in Chennai, India who despite the challenges associated with the recent devastating floods managed to get the production of this first issue out.

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