Review

Advances in materials informatics: a review

Dawn Sivan[1,2], K. Satheesh Kumar[3], Aziman Abdullah[4], Veena Raj[5], Izan Izwan Misnon[1,2], Seeram Ramakrishna[6], and Rajan Jose[1,2,*]

[1] *Faculty of Industrial Sciences and Technology, Universiti Malaysia Pahang Al-Sultan Abdullah, 26300 Kuantan, Pahang, Malaysia*

[2] *Center for Advanced Intelligent Materials, Universiti Malaysia Pahang Al-Sultan Abdullah, 26300 Kuantan, Pahang, Malaysia*

[3] *Department of Future Studies, University of Kerala, Kariavattom, Thiruvananthapuram, Kerala 695581, India*

[4] *School of Computing, Universiti Malaysia Pahang Al-Sultan Abdullah, 25000 Pekan, Malaysia*

[5] *Faculty of Integrated Technologies, Universiti Brunei Darussalam, Gadong, Bandar Seri Begawan BE1410, Brunei*

[6] *Department of Mechanical Engineering, Centre for Nanotechnology and Sustainability, Faculty of Engineering, National University of Singapore, Singapore 117576, Singapore*

ABSTRACT

Materials informatics (MI) is aimed to accelerate the materials discovery using computational intelligence and data science. Progress of MI depends on the strength of database and artificial intelligence protocols comprising machine learning (ML) and deep learning (DL) frameworks. Conventional ML models are simple and interpretable, relying on statistical techniques and algorithms to learn patterns and make predictions with limited data. Conversely, DL, an advancement of ML, employs mathematical neural networks to automatically extract features and handle intricate data at the cost of data size and computational complexity. This work aims to provide a state-of-the-art understanding of the tools, data sources and techniques used in MI and their benefits and challenges. We evaluate the growth of MI through its subfields and track the main path of its advancement for artificial intelligence-driven materials discovery. The advancements in computational intelligence via machine learning and deep learning algorithms in different fields of materials science are discussed. As a specific example, understanding of materials properties using microstructural images is reviewed. Future demands and research prospects in materials science utilizing materials informatics have also been comprehensively analyzed.

Introduction

Data-driven materials discovery via artificial intelligence (AI) in materials sciences, termed materials informatics (MI) [1], plays a significant role in either discovering new materials with user-defined properties or gaining new knowledge on the properties of the existing materials or both [2–5]. In MI, the data from millions of material structures and compositions can be analyzed quickly using machine learning (ML)

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