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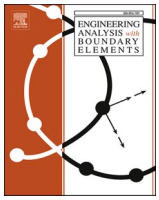

Properties optimisation of nanostructures via machine learning: Progress and perspective

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ABSTRACT

Nanostructures play a vast role in the current Internet of NanoThings (IoNT) era due to remarkable properties and features that precisely impart their desired application functions in catalysis, energy and other fields. The exploration in understanding their minute features caused by the flexibility of compositional and complex atomic arrangement from the synthesis reaction widely opens for the in-depth discovery of their search space such as particle size, morphology and structures that controlled the characteristics. A wide range of possible compositions and various lattice atomic arrangements combined with small particle size distribution and large surface area create grand challenges to copy/differentiate their corresponding specific properties. Thus, the employment of machine learning (ML)-based strategies using the closed-loop experimental data from the nanostructure synthesis to help navigate and optimise for the large classes of data attributes related to the size, morphology and other properties from the trained model are reviewed. The data attributes are assisted by discussions of the selected case studies from the recent literature that highlight different condition nanostructures. The review concludes with a discussion of perspectives on the major challenges in the implementation of ML data-driven design in the field of nanostructure synthesis.

1. Introduction

The current demand on the Internet of NanoThings (IoNT) is to explore more research on the recent progress from supercomputers to smartphones, employing the best small bits of engineered nanomaterials to realise the miniaturised device [1–3]. All the recent nanotechnology advances (*i.e.*, ultrathin designs, intrinsically stretchable nanomaterials and stretchable interconnection designs) involve the fabrication and integration of transdisciplinary modules that use highly customisable nanomaterials and designs [4–9]. For instance, patterned nanomaterials and nanocomposites are frequently utilised to enhance the electrochemically active surface site, which further increases the sensing sensitivity feature of the functional nanodevice. This is to say, the engineered nanomaterials are efficiently produced with tuning structure, composition and functionalisation via preferable bottom-up synthesis to yield unique output properties. Examples include the structural, optical, electrical, magnetic and chemical properties that rely on specific particle characteristics and surface modification from interfacial interaction during synthesis.

It is crucial to have the ability to understand the assembly methodology process for the generation of nanomaterials that are not limited by standard environmental requirements. The operation of synthesised nanoengineered at elevated temperature, pressure and radiation conditions, especially in the future photonic applications is quite challenging. It requires an understanding of nanostructures' behaviour under these extreme conditions. Their level of sensitivity, robustness, and unique property signatures are derived from both the synthesis procedure and accuracy/validation [10–13]. These criteria become more distinctive when a multistep synthesis procedure is involved in attaining the targeted nanostructures. Finding the optimal condition of re-synthesised nanostructures and nanocomposites with a high yield of morphology and monodispersed remains a challenge. Experimentation alone is inadequate to achieve desired structures under finite resources and an appropriate time span. To this end, there is an unprecedented need to access information based on the synthesis method chosen and growth capability for further comprehensive multimodal information of the as-synthesised nanomaterials coupled with modern data analysis techniques (*e.g.*, machine learning and deep learning) [14–16]. This will

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