

Artificial Intelligence for Designing Materials with Improved Performance

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Abstract

To improve the performance of any materials system, i.e. to improve several properties simultaneously, the constituents and the processing parameters must be chosen judiciously. The choice of the parameters for achieving optimum performance of the systems is difficult to arrive experimentally, as the process becomes expensive and laborious.

In silico approaches hold promise for searching the composition and process parameters for achieving the target performance. For designing materials computationally, artificial intelligence and machine learning approaches are implemented to map the hidden relationship between the variables of any complex, nonlinear materials system, and identify the important parameters controlling the final outcome, using available information of the system in a statistically robust and physically meaningful manner. The data-driven relations are used as the objective functions for the optimization processes in single or multi-objective mode, using metaheuristic algorithms, for searching solutions with improved performance.

This talk will provide an overview on the various applications of artificial intelligence tools for modelling and optimization of materials system for designing newer materials.



Dr. Shubhabrata Datta is Research Professor in Mechanical Engineering of SRM Institute of Science and Technology, Kattankulathur, Chennai, India, His research interest is in the domain of design of materials using artificial intelligence and machine learning techniques. Dr. Datta has more than 150 publications in journals and peer-reviewed conference proceedings. Eleven of his graduate students have been conferred with PhD degree. He was bestowed with the Exchange Scientist Award from Royal Academy of Engineering, UK and worked in the University of Sheffield, UK. He also worked in Dept of Materials Science and Engineering, Helsinki University of Technology, Finland, Dept of Materials Science and Engineering, Iowa State University, Ames, USA and Heat Engineering Lab, Dept of Chemical Engineering, Åbo Akademi University, Finland as Visiting Scientist. He is a

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