CONFERENCIA

CENIM
Centro Nacional de Investigaciones Metalúrgicas

Beyond High throughput: Optimal Computational Materials Discovery

Raimundo Arroyave. Department of Materials Science & Engineering Texas A&M University

8 de junio 2017
12:30h

Sala de Confe-rencias del CENIM

Avda. Gregorio del Amo, 8
28040 Madrid

Raymundo Arroyave is a Professor in the Department of Materials Science and Engineering at Texas A&M University. His interests are computational thermodynamics and kinetics of materials, computer-aided materials design and optimal materials discovery. He has published over one hundred publications and currently serves as Chair of the Functional Materials Division of TMS.

The goal-oriented discovery of materials requires the identification of the composition and process history necessary to achieve specific multi-scale structural features that in turn bring about the desired properties. To accelerate the materials discovery process, high-throughput (HT) computational and experimental methods have been proposed. Unfortunately, current HT computational and experimental approaches have severe limitations as they: (1) are incapable of dealing with the high dimensionality (composition, configurational, and microstructural degrees of freedom) and complexity (e.g., multi-physics) of the materials design space; (2) employ hardcoded workflows and lack flexibility to iteratively learn and adapt based on the knowledge acquired to assure balanced exploration and exploitation of the materials design space; (4) are suboptimal in resource allocation as experimental decisions do not account for the cost and time of experimentation.

In this talk, we present some preliminary work in which we have adapted ideas from fields as diverse as Artificial Intelligence, Optimal Experimental Design, Global Optimization and Game Theory to develop a framework capable of optimally exploring the materials design space in order to attain an optimal materials response. Specifically, we use variants of the Efficient Global Optimization algorithm to deploy an autonomous computational materials discovery platform capable of performing optimal sequential computational experiments in order to find optimal materials. We demonstrate single and multi-objective optimization and use the so-called MAX phases as examples. Moreover, we show how this framework can be made robust against selection of non-informative features by using so-called Bayesian Model Averaging approaches.

Vicedirección de Comunicación y Formación. conforma@cenim.csic.es Telf.: 91-5538900 Ext.277

CENIM Centro Nacional de Investigaciones Metalúrgicas
GOBIERNO DE ESPAÑA MINISTERIO DE ECONOMÍA, INDUSTRIA Y COMPETITIVIDAD
CSIC