DE GRUYTER

COMPUTATIONAL INVESTIGATIONS ON THE PROPERTIES AND APPLICATIONS OF HIGH ENTROPY ALLOYS

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DESCRIPTION

In the past few years, an emerging/advanced material – the high entropy alloy (HEA) – has been the subject of metal alloy investigations. HEAs are disordered multicomponent materials of five or more components with almost similar compositions. They usually exist as a single phase which is a result of their stability due to the configurational entropy. The composition requirement and the numerous possible combinations of elements in the periodic table signify a broad opportunity for research and discovery of functional materials based on HEA. However, it also entails the complexity and the challenging task to investigate them computationally and experimentally. In the view of computational materials science, such difficulty could be addressed by improving existing techniques, combining several approaches, and developing new methods. Furthermore, it is possible to employ machine learning algorithms and utilize materials database to investigate HEAs.

It is the aim of this special issue to compile and highlight scientific works that employed computational techniques to study the properties and applications HEAs. It will also give insights into how computational approaches and techniques contribute to the understanding and investigations of such complex materials. We will invite investigators to contribute to this special issue with original research articles and review articles on the relevant advanced science and technologies. Potential topics include but are not limited to the following issues:

- Investigations on HEAs using density functional theory, molecular dynamics, Monte Carlo simulations, machine learning, etc.
- Applications of HEAs as catalyst, sensor, energy material, storage material, permeable material, etc.
- Ceramic, metallic, semiconductor HEAs
- Processes (corrosion, oxidation, diffusion of atoms, reactions, etc.) involving HEAs
- Properties (electronic, structural, stability, mechanical, etc.) and designs of HEAs

PUBLICATION SCHEDULE / HOW TO SUBMIT

All papers will go through the ***Open Physics***' high standard, quick, fair, and comprehensive peer-review procedure. Before submission authors should carefully read the Instructions for Authors. Prospective authors should submit an electronic copy of their complete manuscript through the journal Manuscript Tracking System at http://www.editorialmanager.com/openphys, according to the following timetable:

Open for submissions: 1st November, 2023
Paper submission deadline: 31st March, 2024

When entering your submission please choose the option type of an article: "Computational invest. on the propt. and appl. of high entropy alloys". Submissions for the special issue are now open. In case of any technical problems, please contact the Managing Editor of Open Physics: **Juliusz Skoryna, Ph.D.,** Juliusz.Skoryna@degruyter.com