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Electronic Structure and Modeling of Materials

Guest Editor:

Dr. Titus Sandu
National Institute for Research and Development in Microtechnologies, IMT Bucharest, 077190 Voluntari, Romania

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Message from the Guest Editor

In this Special Issue, we present various facets in computational material science as tools for the quantitative and qualitative description, and characterization of materials, and for uncovering new ones with new functionalities. Ab initio methods like state-of-the-art density functional theory with its many extensions are applicable below the 1 nm scale. Other methods, empirical and/or semiempirical but still atomistic, are successful for the description and characterization of materials at much larger scales. These successive scales and their specifics define the stages of a multiscale approach that is often needed in material sciences since many physical processes manifest at more than one scale. In this call, we welcome contributions in the field of computational materials that may entail approaches from the atomic to the continuum level. However, special attention will be paid to atomistic methods, where modern approaches like machine learning may lead to meaningful model parametrizations, to data-dimensionality reduction, and to property prediction. Practical examples of present interest such as perovskites or 2D materials will have an important role.

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Editor-in-Chief

Prof. Dr. Maryam Tabrizian
1. Department of Biomedical Engineering, Faculty of Medicine and Health Sciences, McGill University, Montreal, QC H3A 2B6, Canada
2. Faculty of Dentistry and Oral Health Sciences, McGill University, 3640 Rue University, Montreal, QC H3A 0C7, Canada

Message from the Editor-in-Chief

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Contact Us

Materials Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
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𝕏@Materials_Mdpi