DESCRIPTION

Aims and Scope:

The aim of the journal is to publish papers that advance the field of computational materials science through the application of modern computational methods alone or in conjunction with experimental techniques to discover new materials and investigate existing inorganic materials, such as metals, ceramics, composites, semiconductors, nanostructures, 2D materials, metamaterials, and organic materials, such as polymers, liquid crystals, surfactants, emulsions, and also hybrid materials combining both inorganic and organic components such as polymer nanocomposites, nanocrystal superlattices or surfactant nanoparticle mixtures.

Papers that report on the development of new methods or the enhancement of existing approaches are of interest.

The scope of the journal includes: obtaining new or enhanced insights into material behavior, properties and phenomena, predicting structure-property relationships for new materials in conjunction with data informatics, novel capabilities of computational tools, technical software and shareware, or cyberinfrastructures.

Contributions are accepted in the form of critical reviews, articles, letters and perspectives. Occasional special issues will be organized around a particular theme and some of these will be guest edited.

Not all topics that potentially fall under the category of computational materials science will be considered; to find out more please visit the Guide for Authors.

AUDIENCE

Materials scientists, physicists, chemists, computer scientists, engineers.

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