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Computational Materials Science

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 investigate existing inorganic and organic materials as well as to discover new materials. Papers that report on the development of new methods or the enhancement of existing approaches are of particular 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.



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