COMPUTATIONAL MATERIALS SCIENCE

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.

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disease and surrounding forest compositions, Mendeley Data, v1, 2015. https://doi.org/10.17632/
xw98nb39r.1.
Reference to software:
K. Lipnikov, R. Garimella, C. Xu, D. Moulton, S. Karra, S. Painter, E. Jafarov, S. Molins, Advanced
Terrestrial Simulator (ATS) v0.88 (Version 0.88), Zenodo, March 25, 2020. https://doi.org/10.5281/
zenodo.3727209.

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