International Journal of
Molecular Sciences

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Computational Approaches in Materials Science

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Message from the Guest Editors

This Special Issue covers recent research topics and review articles on the development and application of computational and theoretical approaches in the design and rationalization of advanced materials, including synthetic and biopolymers and other organic and inorganic components. Original research works or timely reviews privileging theoretical studies or engaging the combination with an experimental part are welcome. Topics include but are not limited to the development and validation of modeling and simulation procedures (atomistic and coarse-grained); quantum, ab-initio, and molecular dynamics; ab-initio and semi-empirical methods; density functional theory; quantum mechanics/molecular mechanics; prediction methods for macromolecular structures; and dynamics and machine-learning approaches.

Deadline for manuscript submissions:
closed (20 October 2019)

mdpi.com/si/24396

Special Issue

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