

## Special Issue

# Computational Approaches in Materials Science

### 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.

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### Guest Editors

Prof. Dr. Alberto Pais

Dr. Sandra Nunes

Dr. Tânia Cova

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### Deadline for manuscript submissions

closed (20 October 2019)



## International Journal of Molecular Sciences

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Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland  
Tel: +41 61 683 77 34  
[ijms@mdpi.com](mailto:ijms@mdpi.com)

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### Message from the Editor-in-Chief

The International Journal of Molecular Sciences (*IJMS*, ISSN 1422-0067) is an open access journal, which was established in 2000. The journal aims to provide a forum for scholarly research on a range of topics, including biochemistry, molecular and cell biology, molecular biophysics, molecular medicine, and all aspects of molecular research in chemistry. *IJMS* publishes both original research and review articles, and regularly publishes special issues to highlight advances at the cutting edge of research. We invite you to read recent articles published in *IJMS* and consider publishing your next paper with us.

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### Editor-in-Chief

Prof. Dr. Maurizio Battino

Department of Odontostomatologic and Specialized Clinical Sciences,  
Sez-Biochimica, Faculty of Medicine, Università Politecnica delle  
Marche, Via Ranieri 65, 60100 Ancona, Italy

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