



## New Advances in Density Functional Theory and Its Application

Guest Editors:

**Prof. Dr. Juan-Carlos Sancho-García**

**Prof. Dr. Emilio San-Fabián Maroto**

**Prof. Dr. José-Manuel García De la Vega**

**Prof. Dr. Karlheinz Schwarz**

Deadline for manuscript  
submissions:

**closed (31 May 2020)**

### Message from the Guest Editors

Dear Colleagues,

This Special Issue will consist of selected excellent papers from the “18th International Conference on Density-Functional Theory and its Applications”, which will be held in Alicante (Spain) from 22 to 26 July 2019.

This worldwide used theory constitutes one of the most applied quantum theories developed so far and has outstanding applications in many scientific fields. This Special Issue is dedicated to demonstrating how recent advances can pave the way towards cutting-edge applications for a better and more sustainable future.

We invite contributors to this edition to submit and present papers in a variety of fields, from concepts and developments to applications. Papers may report on original research, discuss methodological aspects, present new applications, and review the current state-of-the-art, or offer perspectives or future prospects for the field. The papers will undergo a strict peer-review process and, when accepted, be published to widely disseminate their contents and results.

Prof. Drs. Juan-Carlos Sancho-García, Emilio San-Fabián, José-Manuel García de la Vega, and Karlheinz Schwarz

*Guest Editors*





an Open Access Journal by MDPI

## Editor-in-Chief

### Prof. Dr. Ali Cemal Benim

Center of Flow Simulation (CFS),  
Department of Mechanical and  
Process Engineering, Duesseldorf  
University of Applied Sciences, D-  
40476 Duesseldorf, Germany

## Message from the Editor-in-Chief

You are invited to submit the results of your research for consideration and publication in *Computation*, an international open access journal, which is published monthly online by MDPI.

The editorial board and staff of *Computation* are dedicated to establishing a benchmark journal for the world scientific and engineering communities for original research articles, reviews, conference proceedings (i.e., peer reviewed full articles), and communications, in the cutting-edge areas of computational biology, computational chemistry, and computation in engineering.

## Author Benefits

**Open Access:** free for readers, with article processing charges (APC) paid by authors or their institutions.

**High Visibility:** indexed within Scopus, ESCI (Web of Science), CAPlus / SciFinder, Inspec, dblp, and other databases.

**Journal Rank:** JCR - Q2 (*Mathematics, Interdisciplinary Applications*) / CiteScore - Q2 (*Applied Mathematics*)

## Contact Us

---

*Computation* Editorial Office  
MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland

Tel: +41 61 683 77 34  
www.mdpi.com

mdpi.com/journal/computation  
computation@mdpi.com  
X@ComputationMDPI