

## Special Issue

# New Advances in Density Functional Theory and Its Application

### Message from the Guest Editors

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

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)



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## About the Journal

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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.

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