Special Issue

Modeling Transition-Metal Systems: Emerging Developments and Applications

Message from the Guest Editors

Transition-metal compounds are at the core of several cutting-edge technologies, including the advanced energy, electronics, sensing, actuation, and functionalization. This Special Issue aims to attract leading researchers in the field of ab initio modeling of strongly correlated materials. The main objectives are to review the beyond-DFT computational approaches used to model correlated materials and to discuss some of the most recent developments; to illustrate significant advances on the calculation of relevant properties for materials characterization and technological applications; and to discuss and clarify some of the most important aspects of the physics of these systems. Particular emphasis will be given to methodological and application-related investigations discussing:

- The effects of correlation on phase stability and vibrational properties;
- The interplay among crystal structure, magnetic orders, and conduction properties;
- Magnetism and electronic conduction in 2D transition-metal and rare-earth compounds;
- Strong correlation and photo-/electrochemical properties.

Guest Editors

Dr. Matteo Cococcioni

The Physics Department, The University of Pavia, Pavia, Italy

Dr. Andrea Floris

School of Chemistry, College of Science, University of Lincoln, Lincoln LN6 7TS, UK

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Applied Sciences
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
applsci@mdpi.com

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Message from the Editor-in-Chief

As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal Applied Sciences has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multi-dimensional network.

Editor-in-Chief

Prof. Dr. Giulio Nicola Cerullo
Dipartimento di Fisica, Politecnico di Milano, Piazza L. da Vinci 32, 20133 Milano, Italy

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