



## Molecular Simulations of Functionalized Nanoscale Materials

Guest Editors:

**Dr. Paul Mulheran**

Department of Chemical and  
Process Engineering, University  
of Strathclyde, Glasgow G1 1XJ,  
UK

**Dr. Giorgia Brancolini**

Consiglio Nazionale delle  
Ricerche, CNR NANO - Institute  
Nanoscience, Center S3, via G.  
Campi 213/A, 41125 Modena,  
Italy

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submissions:

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### Message from the Guest Editors

Dear Colleagues,

Well-designed molecular simulations can give atomistic insight into the interactions between a biomolecule and an inorganic/organic surface, revealing details that cannot be accessed through experiment alone. In turn, experiments can validate some key aspects of the simulation to build confidence in the theoretical predictions. This synergy between experiment and simulation can be harnessed to optimize the design of functionalized nanoscale systems, and indeed provide rational design tools to create new technologies.

In this Issue, we bring together research at the interface between modelling and experiment, where molecular simulation plays an important role in the scientific discovery and development of functionalized nanoscale materials. The systems of interest include, amongst others: Targeted drug delivery; Novel therapeutics and vaccines; Imaging and diagnostics; Biosensors; Industrial catalysis.

Full papers and short communications covering methodological and theoretical aspects, as well as interdisciplinary approaches underlying the potential interpretation of experimental data and applications are all welcome.

Dr. Paul Mulheran  
Dr. Giorgia Brancolini





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Conocimiento s/n, 18100 Armilla,  
Granada, Spain

## Message from the Editor-in-Chief

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*International Journal of Molecular  
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MDPI, Grosspeteranlage 5  
4052 Basel, Switzerland

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