



## Modelling and Simulations in Polymer Surface Chemistry

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submissions:

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### Message from the Guest Editors

This Special Issue focuses on theoretical models and computational studies of polymers' surfaces and interfaces. The surfaces of polymers and composites are of critical importance for numerous technological applications: sensors, electrochemistry, coating, energy and biological applications, etc. It is an intrinsically multidisciplinary area where chemical and material syntheses are in close contact with nanotechnology, theoretical chemistry and physics.

Papers are sought that relevance to this field, focusing on modelling, theoretical and computational work, with or without supporting experimental results.

The scope of this Special Issue is wide and we are looking forward to receive contributions on simulations of characterization techniques or models of functionalization of polymers' surfaces, as well as theoretical approaches that suggest the novel application of polymers' surfaces in fields including electrochemistry, catalysis, coating and corrosion protection, drugs delivery, sensing and photochemistry. Simulations of self-healing polymers and polymers' degradation are also relevant when they specifically address the role of interfaces and surfaces.





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## Message from the Editor-in-Chief

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I would like to invite you to contribute to the success of the journal by sending us your high quality research papers. We would be pleased to welcome you as one of our authors.

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