



Molecular Dynamics Simulation of Polymer for Absorption and Separation Applications

Guest Editors:

Dr. Ioannis Tanis

The Cyprus Institute, Aglantzia,
Cyprus

Prof. Dr. Costas H. Vlahos

Department of Chemistry,
University of Ioannina, Ioannina,
Greece

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Message from the Guest Editors

Adsorption and separation are highly efficient processes that are widely used in diverse applications ranging from wastewater treatment, desalination, and forward and reverse osmosis to natural gas purification and hydrogen storage. Polymer membranes and nanocomposites are a class of materials that are appealing candidates in the aforementioned applications due to their unique attributes, such as the existence of easily modifiable functional groups, as well as their high thermal and mechanical stability. Molecular dynamics simulations constitute an invaluable tool for the study of such processes as they can successfully complement experimental approaches and shed light on mechanism operations at the molecular level, such as polymer-penetrant interactions and penetrant transport in the polymer matrix micro-cavities. On these grounds, this Special Issue invites the submission of manuscripts which present recent developments in this field, through the use of various computational methods. Contributions which present complementary experimental and numerical approaches are particularly welcome.





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Editor-in-Chief

Prof. Dr. Alexander Böker

Fraunhofer-Institut für
Angewandte Polymerforschung,
Lehrstuhl für Polymermaterialien
und Polymertechnologie,
Universität Potsdam,
Geiselbergstraße 69, 14476
Potsdam-Golm, Germany

Message from the Editor-in-Chief

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Contact Us

Polymers Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
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