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Molecular Dynamics Simulation of Polymer for Absorption and Separation Applications

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Deadline for manuscript submissions:
closed (15 January 2024)

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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Message from the Editor-in-Chief

Since its foundation in 2009, *Polymers* has developed into an internationally renowned, extremely successful open access journal. The editorial team and the editorial board dedicatedly combine open-access publishing and high-quality rigorous peer reviewing. The performance of the journal has proven this strategy to be well-suited and highly successful. This is reflected in the increasing impact factor of *Polymers*, the most recent one being 5.0.

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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