

Special Issue

Ion and Molecular Transport in Nanopores/Channels

Message from the Guest Editor

This Special Issue showcases the latest computational advances in understanding and predicting the ion and molecular transport within nanoconfined channels and pores, where fluid, ion, and molecule behavior significantly deviates from bulk phases due to geometric confinement, surface charge, and boundary slip. These phenomena are central to biological processes and membrane separation technology. The Issue invites original research and reviews that use theoretical modeling, advanced simulations, and high-performance computing to reveal underlying transport mechanisms and guide the design of next-generation membranes. Relevant research areas include, but are not limited to, water desalination, gas separation, novel membrane materials, transport mechanisms in confined channels, multiscale simulations, and machine learning applications. Contributions are welcome that employ computational methods like molecular dynamics, ab initio simulations, Poisson–Nernst–Planck–Stokes theory, and finite element analysis

Guest Editor

Dr. Haiqi Gao

State Key Laboratory of Chemistry and Utilization of Carbon Based Energy Resources, Xinjiang University, Urumqi 830017, China

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Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
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Prof. Dr. José L. Quiles
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