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Special Collection on the Frontiers of Computational Biophysics





Call for Papers

Special Collection on the Frontiers of Computational Biophysics

This Special Collection will explore the frontiers of multiscale modeling from all-atom molecular dynamics and mixed quantum-classical (QM/MM) approaches to coarse-grained and mesoscale representations of biomolecules into the cell environment, exploring novel integrative methods that bridge the macromolecular (nm) to sub-cellular (µm) levels. These will include different kinds of phase space sampling, such as Brownian dynamics, other stochastic dynamics and advanced sampling methods. This Special Collection will also comprise emerging computational approaches harnessing artificial intelligence and deep learning, which further empower computational biophysics toward new frontiers.

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Topics

Molecular Dynamics – Mixed QM/MM Approaches – Coarse-Grained – Mesoscale & Cell Modeling – Brownian Dynamics – Protein Topology & Elastic Network Modeling – Protein Design – Artificial Intelligence in Biophysics – Protein Prediction – Cryo-EM Processing – Integrative Modeling – Electrostatics Simulations – Polarizable Models – Biophysics of Drug Design – Biomolecular Visualization – Nucleic Acids – Membranes – Macromolecular Machines – Receptors & Channels





The <u>Editorial Board</u> would like to cordially invite you to contribute with a research article or a review/perspective for our special edition.

QRB Discovery publishes new developments in the field of experimental and computational biophysics. Articles report on significant physical observations of relevance to biological systems, both experimental and theoretical, that may point towards an exciting direction, rather than the presentation of a traditional comprehensive study.

Your paper will go through peer review and we encourage you to contact biophysics@cambridge.org if you want to discuss your submission.

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