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## **Special Collection on the Frontiers of Computational Biophysics**

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# **Call for Papers**

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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 ( $\mu$ m) 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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