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Symmetry in Molecular Dynamics

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Message from the Guest Editor

Molecular dynamics simulations have been extensively tested to reproduce the dynamical evolution of intrinsically disordered systems. At present, the correct model of highly symmetric molecular aggregates is a challenge. In particular, the influence of symmetry in protein dynamics is known, especially in circularly symmetric homo-oligomeric proteins. Indeed, many supramolecular structures are symmetric in their nature. Among them, homo-oligomeric ion channels are highly symmetric, which dramatically decreases conformational space and facilitates the building of homology models. However, in standard molecular dynamics (MD) simulations, channels deviate from ideal symmetry, thus complicating the refinement of the built models. Symmetry-constrained MD simulations can deeply improve their accura

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Message from the Editor-in-Chief

Symmetry is ultimately the most important concept in natural sciences. It is not surprising then that very basic and fundamental research achievements are related to symmetry. For instance, the Nobel Prize in Physics 1979 (Glashow, Salam, Weinberg) was received for a unified symmetry description of electromagnetic and weak interactions, while the Nobel Prize in Physics 2008 (Nambu, Kobayashi, Maskawa) was received for the discovery of the mechanism of spontaneous breaking of symmetry, including CP symmetry. Our journal is named *Symmetry* and it manifests its fundamental role in nature.

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