SYMMETRY-CONSTRAINED MOLECULAR DYNAMICS

ANDREW WHITE, SAM COX, *Chemical Engineering, University of Rochester, Rochester, NY, USA*.

Molecular dynamics is a popular tool for molecular structure prediction, but the application into crystal structures has been limited by the inability to treat point group symmetries. For this reason, many space groups are inaccessible in typical molecular dynamics, though the inaccessible space groups are often desirable. We propose symmetry-constrained molecular dynamics as a new approach to address these space groups. This method allows all point group symmetries to be accessible in molecular dynamics simulations. Because there is a small number of possible space groups, these can be enumerated, as shown in this work. Spectroscopy and molecular dynamics are mutually beneficial techniques to understand systems more fully, and spectroscopy has deep roots in symmetry, as symmetries give insight into chemical shift prediction, for molecules and crystals. Therefore, this work bridges the gap between spectroscopy and structure prediction by molecular dynamics.