Multiscale Modeling Study for High Temperature Piezocrystals

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Piezoelectric ceramics based on the pervoskite system are widely used as sensors and actuators. In most applications, the need for actuation and sensing over a broad temperature range is essential. Systems with enhanced piezoelectric activity and elevated temperature have redirected effort on single crystals in relaxor-PT systems.

In this work, the high-temperature pervoskite ferroelectrics in the solid solution (1-x)$BiScO_3$-x$PbTiO_3$ are investigated through the multiscale modeling simulations. Starting with quantum mechanical simulations, first principles calculations provide us the fundamental information, including the ground states atomic structures and interatomic forces, ferroelectric double-well energy surfaces, dynamical effective charges, dielectric constants and phonon spectra. A transferable atomistic model is developed through optimization of empirical interatomic potentials based on first principles data. With the interatomic potentials, molecular dynamics simulations are applied to study the ferroelectric properties of BS-PT under external loading, including a wide range of pressures, temperatures and with different compositions. An optimized design of the solid solution (1-x)$BiScO_3$-x$PbTiO_3$ is obtained for actuation and sensing applications in extreme environment.

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