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Thermo-Electromechanical Coupling Effects on Ferroelectric Perovskites XIAOWEI ZENG, George Washington University, JAMES LEE, George Washington University, YOUPING CHEN, George Washington University — We are investigating the thermo-electromechanical coupling effects on ferroelectric perovskite materials. This work is based on a shell model potential with parameters obtained from first-principles calculation. Molecular dynamics simulations are performed to investigate the dynamic response of the ferroelectric perovskites under thermal, mechanical and electric loadings. The phenomena of finite temperature phase transitions and polarization reorientation are observed. The temperature-pressure phase diagram is also obtained.

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