Understanding the physical chemistry properties of $Ba_xSr_{1-x}TiO_3$ using ReaxFF based Molecular Dynamics Simulations

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Project Summary: An understanding of the surface chemistry of substrates used as support for 2D-chalcogenide growth is essential for controlling the synthesis of these materials. As such, we need computational methods that can be used to study the reaction dynamics of these support materials. The ReaxFF method – which allows for relatively large (>> 10,000 atoms), long-time (>> 1 nanoseconds) fully reactive, fully dynamics simulations of complex materials and their interfaces allows for atomistic-scale simulations that can directly connect to experimental synthesis efforts. In order to expand the ReaxFF capability for support material simulations, we have extended a previously developed ReaxFF parameter set for $BaTiO_3$ to $SrTiO_3$ (STO) – a highly relevant support material for 2D-chalcogenide growth. This ReaxFF description can be used for any Ba/Sr ratio and can describe key surface chemistry – including water vapor and oxidation/reduction reactions at the STO surface. These ReaxFF parameters were validated against Density Functional Theory (DFT) data and was validated be studying ferroelectric transitions in mixed $Ba/SrTiO_3$ materials.

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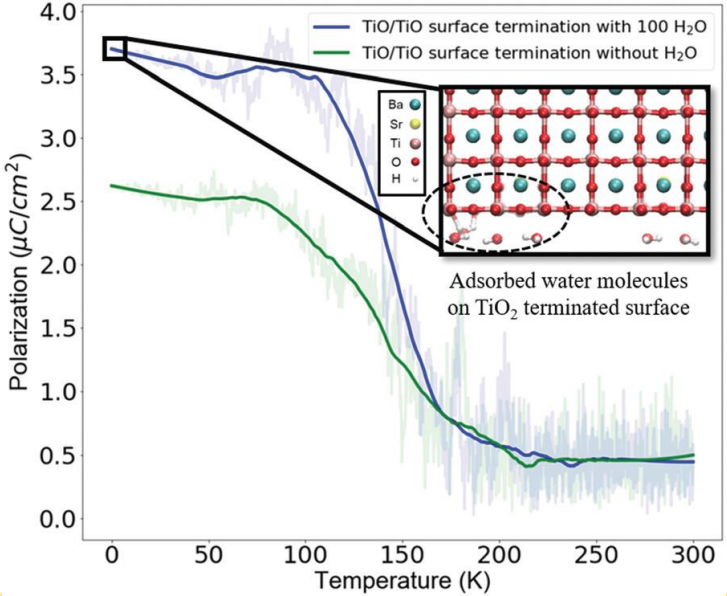
2DCC Role: This project is associated with the 2DCC target of developing new computational capabilities for simulating 2D-materials and support materials associated with the growth of these materials.



Effects of the water interaction with TiO_2 terminated surfaces of a 14.6 nm BSTO slab on the polarization. The charge screening induced by adsorption of H_2O molecules on TiO_2 terminated surfaces leads to an increased amount of initial polarization from 2.6 mC cm^{-2} (green line) to 3.7 mC cm^{-2} (blue line).