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Effects of ferroelectric polarization on surface phase diagram: an evolutionary algorithm study of the $BaTiO_3$(001) surface[1] PENGCHENG CHEN, YONG XU, NA WANG, Tsinghua University, ARTEM R. OGANOV, Stony Brook University, WENHUI DUAN, Tsinghua University — We have constructed the surface phase diagram of the $BaTiO_3$(001) surface by employing an evolutionary algorithm for surface structure prediction, where the ferroelectric polarization is included as a degree of freedom. Among over 1000 candidate structures explored, a surface reconstruction of (2×1)-TiO is discovered to be thermodynamically stable and have the *p2mm* plane group symmetry as observed experimentally. We find that the influence of ferroelectric polarization on the surface free energy can be either negligibly small or sizably large (over 1 eV per (2×1) supercell), depending strongly on the surface structure and resulting in a significant distinction of surface phase diagram with varying ferroelectric polarization. It is therefore feasible to control the surface stability by applying an external electric field. Our results may have important implications in understanding the surface reconstruction of ferroelectric materials and tuning surface properties.

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