

**High-throughput prediction of oxygen vacancy defect migration near
misfit dislocations in SrTiO₃/BaZrO₃ heterostructures**

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Supporting Information

Figure 1. Visualization of a single atomic layer for SrO–ZrO₂ and TiO₂–BaO interfaces. (a) SrO side of SrO–ZrO₂ (b) ZrO₂ side of SrO–ZrO₂ (c) TiO₂ side of TiO₂–BaO (d) BaO side of TiO₂–BaO. Interface orientation is same for all materials as given in (c). Atomic color scheme is given below the figure panel.

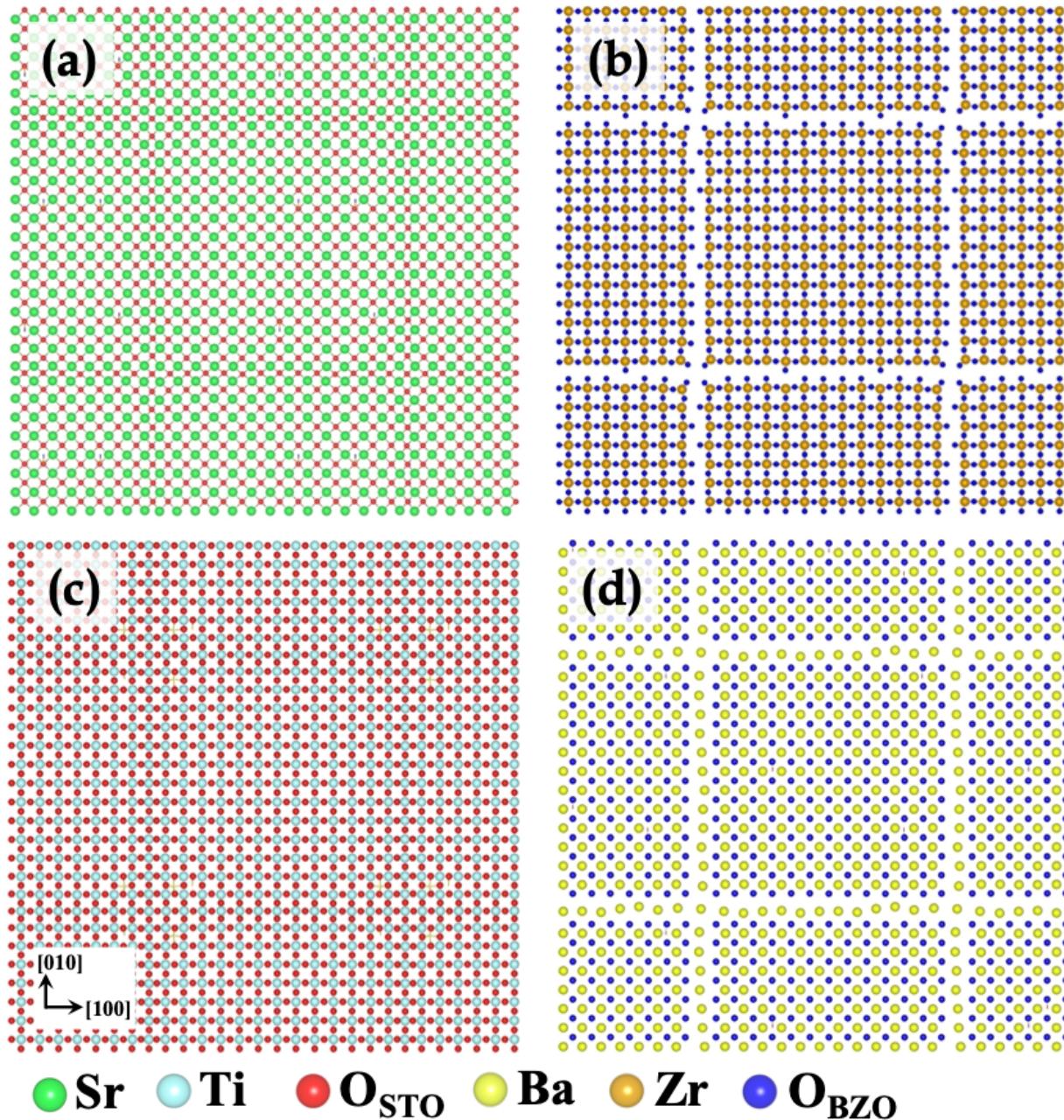


Figure 2. Visualization of a single atomic layer for SrO–BaO and TiO₂–ZrO₂ interfaces. (a) SrO side of SrO–BaO (b) BaO side of SrO–BaO (c) TiO₂ side of TiO₂–ZrO₂ (d) ZrO₂ side of TiO₂–ZrO₂. Interface orientation is same for all materials as given in (c). Atomic color scheme is given below the figure panel.

