

Supporting Information

Thickness-dependent electronic and optical properties of two-dimensional perovskite
oxide films: A first-principles study

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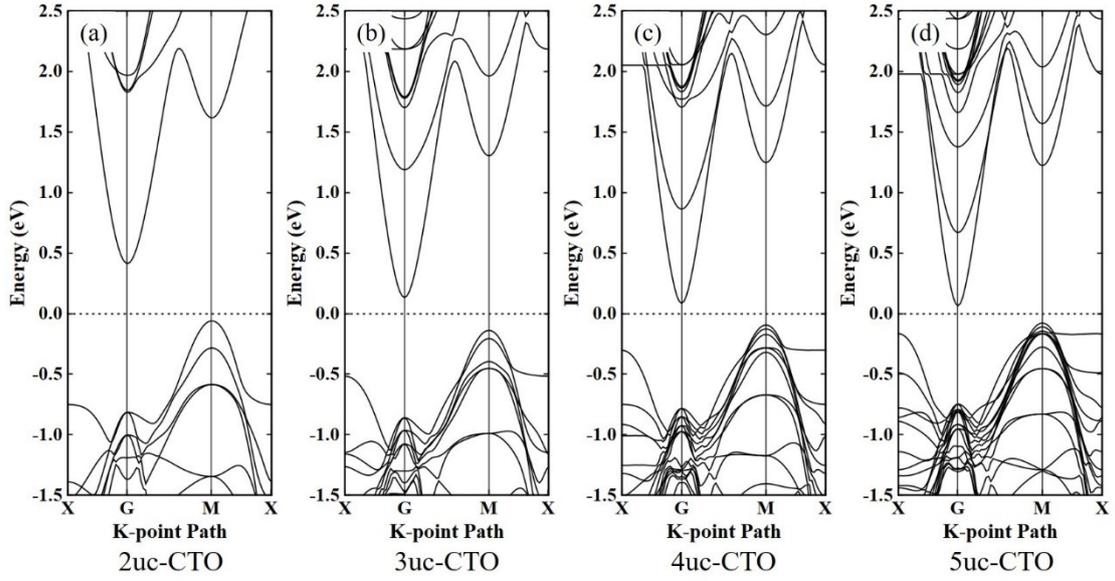


Fig. S1. Energy bands of 2D CTO films with different thickness: (a) 2uc-CTO, (b) 3uc-CTO, (c) 4uc-CTO, and (d) 5uc-CTO. The Fermi level (E_f) was set to zero and is indicated by a horizontal dashed line in above and all subsequent energy band structure diagrams.

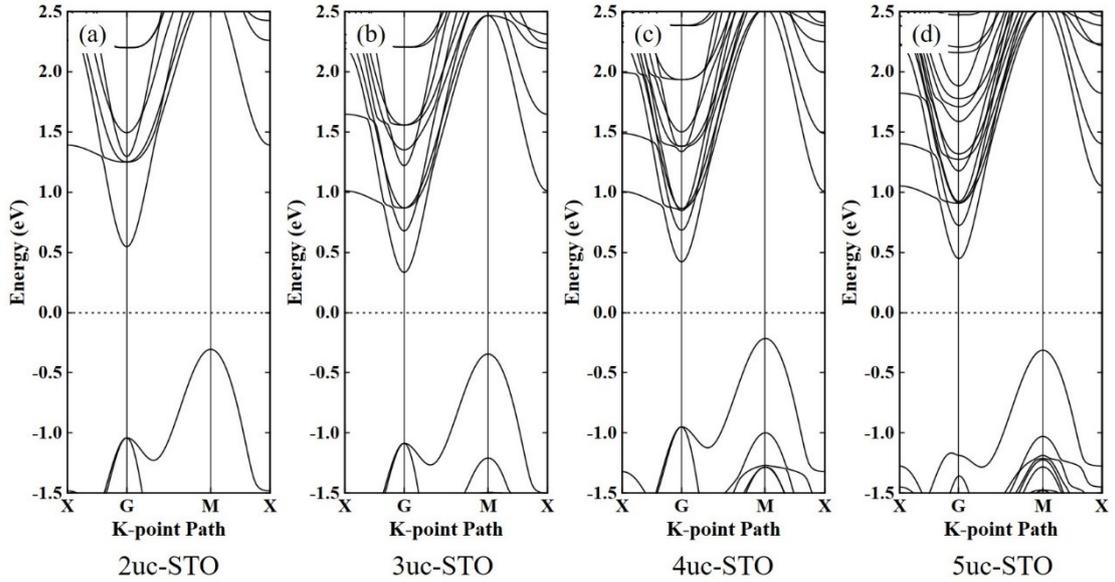


Fig. S2. Energy bands of 2D STO films with different thickness: (a) 2uc-STO, (b) 3uc-STO, (c) 4uc-STO, and (d) 5uc-STO.

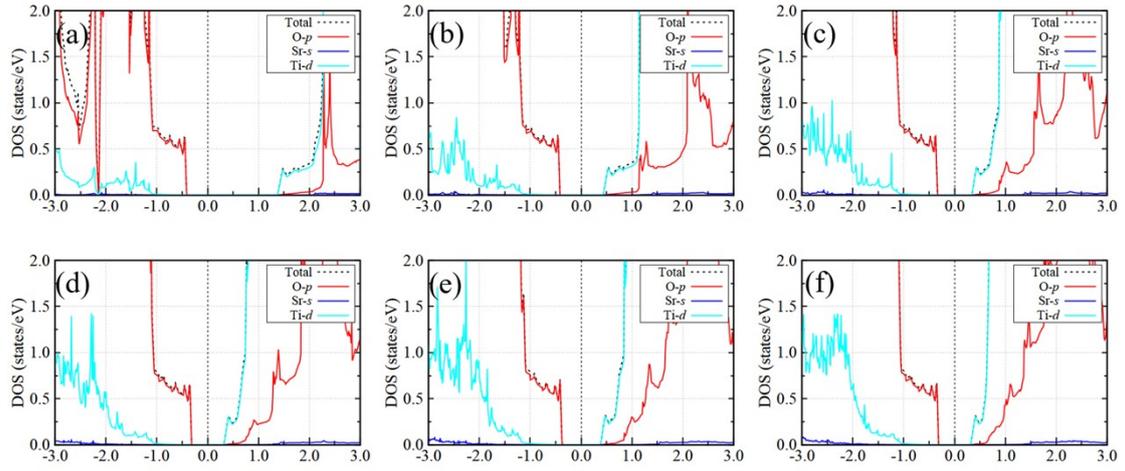


Fig. S3. Element-resolved DOS of 2D STO films with different thickness: (a) 1uc-STO, (b) 2uc-STO, (c) 3uc-STO, (d) 4uc-STO, (e) 5uc-STO, and (f) 6uc-STO.

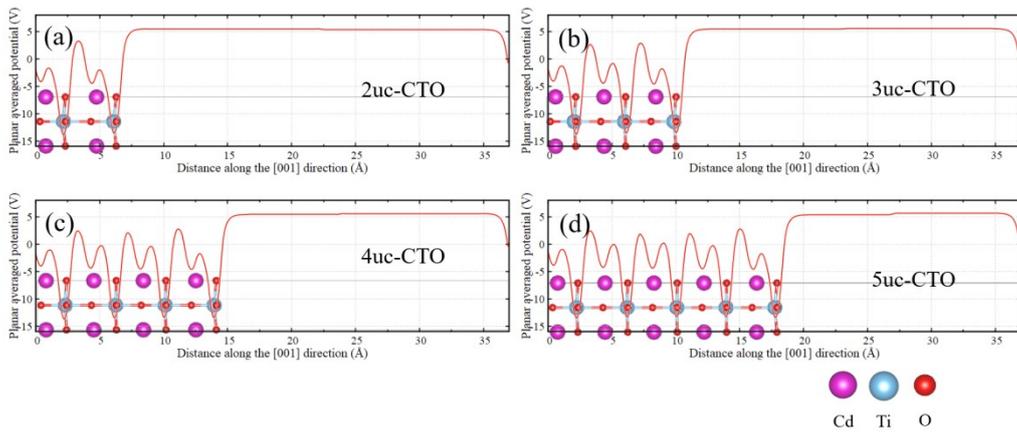


Fig. S4. The planar averaged potential of 2D CTO films: (a) 2uc-CTO, (b) 3uc-CTO, (c) 4uc-CTO, and (d) 5uc-CTO.

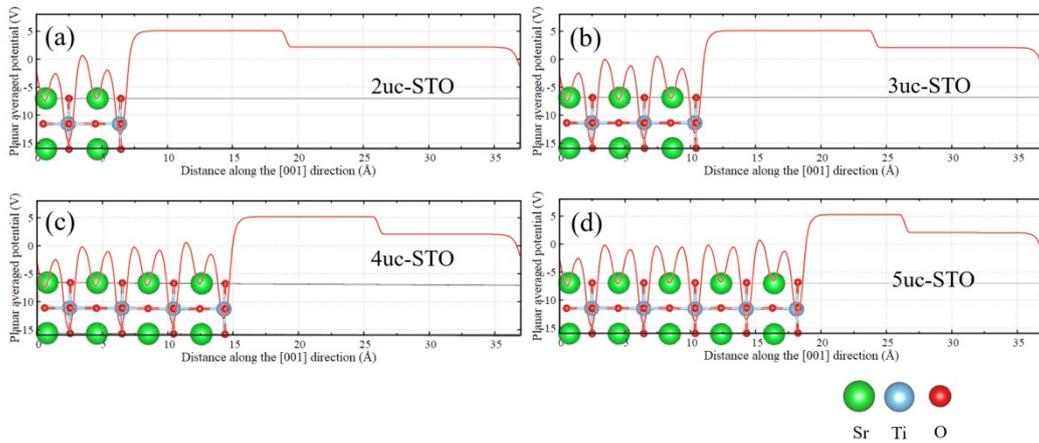


Fig. S5 The planar averaged potential of 2D STO films: (a) 2uc-STO, (b) 3uc-STO, (c) 4uc-STO,

and (d) 5uc-STO.

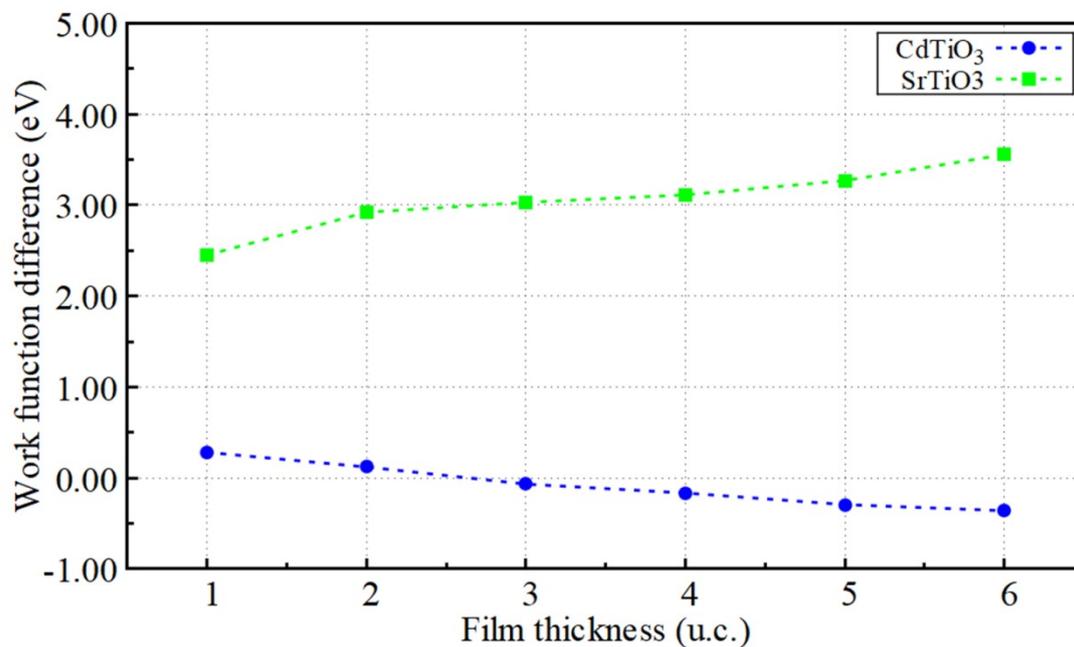


Fig. S6. The variation of the difference in work function between the upper and lower surfaces of CTO and STO films as a function of film thickness.

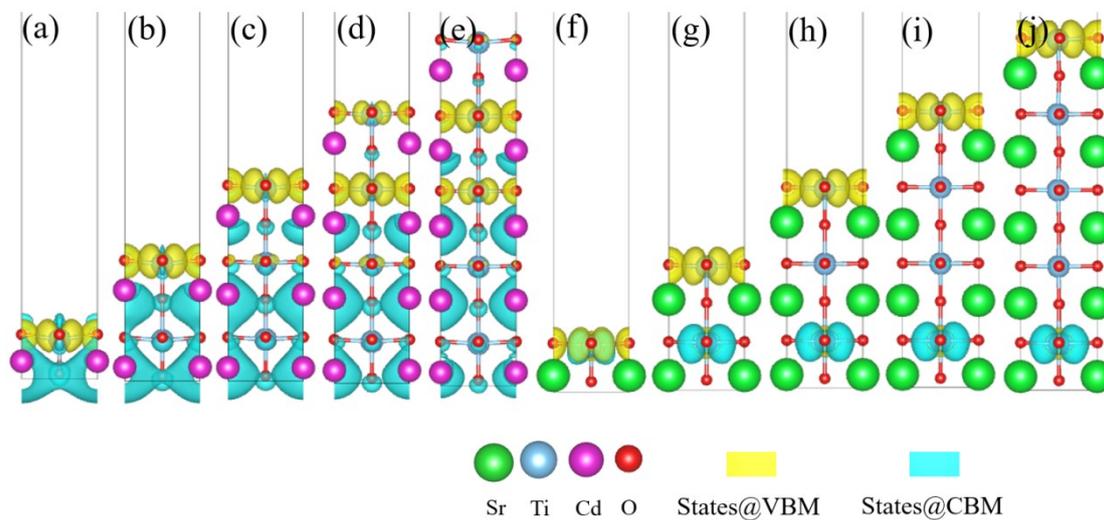


Fig. S7. Side views of the electronic state distributions, projected at VBM and CBM for (a) 1uc-CTO, (b) 2uc-CTO, (c) 3uc-CTO, (d) 4uc-CTO, (e) 5uc-CTO, (f) 1uc-STO, (g) 2uc-STO, (h) 3uc-STO, (i) 4uc-STO, (j) 5uc-STO.

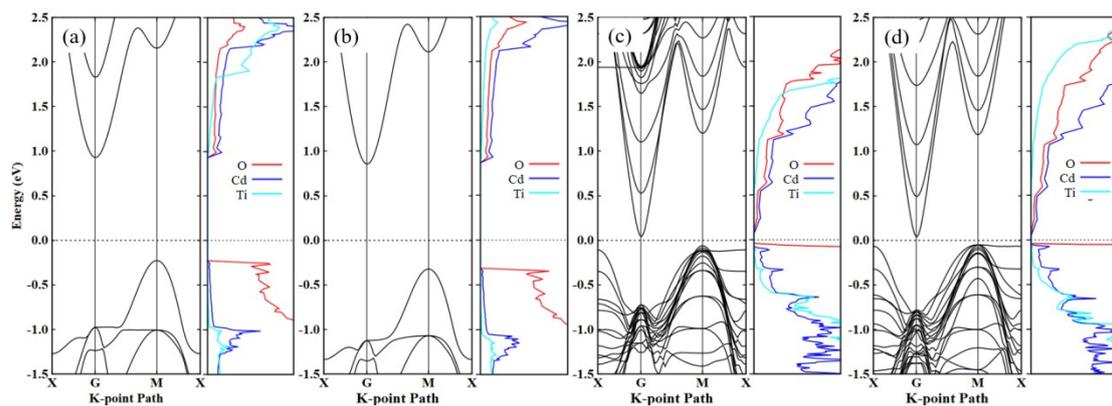


Fig. S8. Band structures and element-resolved DOS of (a) 1uc-CTO without U correction, (b) 1uc-CTO with U correction, (c) 6uc-CTO without U correction, and (d) 6uc-CTO with U correction.

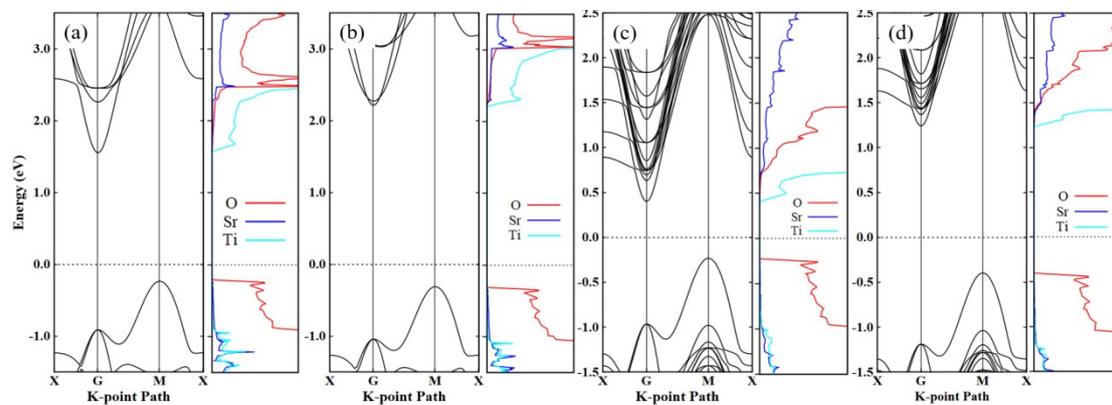


Fig. S9. Band structures and element-resolved DOS of (a) 1uc-STO without U correction, (b) 1uc-STO with U correction, (c) 6uc-STO without U correction, and (d) 6uc-STO with U correction.