

Recruiting Perovskites to Degrade Toxic Trinitrotoluene

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Table S1. Calculated lattice parameters of BTO, BSTO, and STO ideal bulk crystals in $R3m$ space group ($\alpha=90^\circ$) and the (001) $4a_0 \times 4a_0$ surface cell 7-plane slab with the $5a_0$ -wide vacuum gap.

Lattice parameter	Material	BTO	BSTO	STO
a_0 , Å	bulk	4.05 (4.00 ^a)	4.01	3.95 (3.90 ^b)
	surface	4.03	3.97	3.92

^a Experimental lattice constants of BTO were taken from ref.¹.

^b Experimental lattice constants of STO were taken from ref.².

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