SUPPORTING INFORMATION

Property Control from Polyhedral Connectivity in ABO_3 Oxides

Nicholas Wagner,[1] Ram Seshadri,[2] and James M. Rondinelli[1]

[1] *Department of Materials Science and Engineering, Northwestern University, Evanston, IL 60208, USA*

[2] *Materials Department, Materials Research Laboratory, University of California, Santa Barbara, California 93106, USA*

TABLE S1. Available experimental crystal structures for $BaMnO_3$ and $BaTiO_3$.

		M=Ti			M=Mn				
0% Face-sharing		$Amm2$ (#38) $a = 3.9828$ Å, $b = 5.6745$ Å, $c = 5.6916$ Å $\alpha = \beta = \gamma = 90°$							
Atom	Wyck. Site	x	y	z	Atom	Wyck. Site	x	y	z
Ba	2a	0	0	0					
Ti	2b	1/2	0	0.5170					
O(1)	2a	0	0	0.4890					
O(2)	4e	1/2	0.2439	0.7343					
33% Face-sharing		$P6_3/mmc$ (#194) $a = b = 5.7238$ Å, $c = 13.9649$ Å $\alpha = \beta = 90°$, $\gamma = 120°$							
Atom	Wyck. Site	x	y	z	Atom	Wyck. Site	x	y	z
Ba(1)	2b	0	0	1/4					
Ba(2)	4f	1/3	2/3	0.09671					
Ti(1)	2a	0	0	0					
Ti(2)	4f	1/3	2/3	0.84633					
O(1)	6h	0.5185	0.0370	1/4					
O(2)	12k	0.8349	0.6698	0.0802					
50% Face-sharing					$P6_3/mmc$ (#194) $a = b = 5.62732$ Å, $c = 9.20800$ Å $\alpha = \beta = 90°$, $\gamma = 120°$				
Atom	Wyck. Site	x	y	z	Atom	Wyck. Site	x	y	z
					Ba(1)	2a	0	0	0
					Ba(2)	2c	1/3	2/3	1/4
					Mn	4f	1/3	2/3	0.89145
					O(1)	6g	1/2	0	0
					O(2)	6h	0.81323	0.62646	1/4
100% Face-sharing					$P6_3/mmc$ (#194) $a = b = 5.6991$ Å, $c = 4.8148$ Å $\alpha = \beta = 90°$, $\gamma = 120°$				
Atom	Wyck. Site	x	y	z	Atom	Wyck. Site	x	y	z
					Ba	2d	1/3	2/3	3/4
					Mn	2a	0	0	0
					O	6h	0.14950	0.2990	1/4

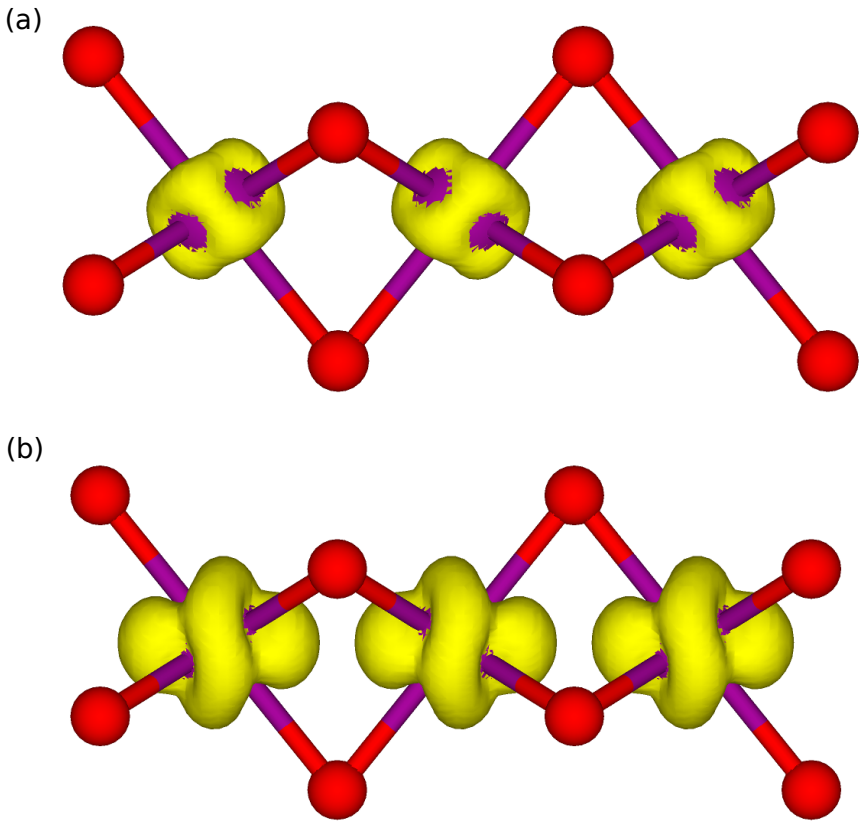

FIG. S1. Density functional theory partial charge density for the (a) valence and (b) conduction bands of the 100% $BaMnO_3$ polymorph. The valence band exhibits e_g^π symmetry whereas the conduction band exhibits a_{1g}^* symmetry. The isosurface levels for the density contours are $0.162\,e\text{Å}^{-3}$ and $0.068\,e\text{Å}^{-3}$ respectively.