Supporting Information: 'Ferroelectric' Metals Reexamined: Fundamental Mechanisms and Design Considerations for New Materials

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Table 1: Comparison between calculated and experimental structural parameters of $R\bar{3}c$ $LiOsO_3$ in the hexagonal setting. The calculated lattice parameters are $a = 5.1091$ Å and $c = 13.0175$ Å, compared with the experimental lattice parameters $a = 5.0638$ Å and $c = 13.2110$ Å. The calculated rotation angle for the OsO_6 octahedra is 23.9°, compared with an experimental value of 24.2°. Experimental data are from Shi, *et al Nature Materials* **12** 1024 (2013).

Atom	Wyckoff site	Theory			Experiment		
		x	y	z	x	y	z
Li	6a	0	0	0.25	0	0	0.25
Os	6b	0	0	0	0	0	0
O	18e	0.6277	0	0.25	0.6298	0	0.25

Table 2: Comparison between calculated and experimental structural parameters of $R3c$ $LiOsO_3$ in the hexagonal setting. The calculated lattice parameters are $a = 5.0421$ Å and $c = 13.2470$ Å, compared with the experimental lattice parameters $a = 5.0456$ Å and $c = 13.2390$ Å. Experimental reference as above.

Atom	Wyckoff site	Theory			Experiment		
		x	y	z	x	y	z
Li	6a	0	0	0.2199	0	0	0.2147
Os	6a	0	0	0.0057	0	0	0
O	18b	0.6701	-0.0311	0.2582	0.6260	-0.0102	0.2525