

Supplementary Information for

“Factors Favoring Ferroelectricity In Hafnia: A First Principles Computational Study”

by

Rohit Batra, Tran Doan Huan, Jacob L. Jones, George Rossetti, Jr. and Rampi Ramprasad

Following document lists the values of relative permittivity and the spontaneous polarization of different phases of hafnia used to construct Fig. 3 in the main article.

Table S1: The elements of relative permittivity and the magnitude of spontaneous polarization of different phases of hafnia under equilibrium, hydrostatically compressed and equibiaxially compressed ($\epsilon = 4.3\%$) states. The polarization values were computed using both the VASP and the ABINIT package (within brackets) to ensure reproducibility. The relative permittivity and the polarization values for Fig. 3(d), (e) and (f) of the main article were obtained by linear interpolation between the equilibrium and the equibiaxially compressed state (with $\epsilon = 4.3\%$).

State	Phase	ϵ_{xx}	ϵ_{yy}	ϵ_{zz}	ϵ_{xy}	ϵ_{xz}	ϵ_{yz}	P ($\mu\text{C}/\text{cm}^2$)
Equilibrium	M	20.63	18.91	15.87	0.00	1.42	0.00	0
	T	140.37	140.37	17.44	0.00	0.00	0.00	0
	P-O1	25.23	23.62	20.30	0.00	0.00	0.00	50(49)
	P-O2	22.40	22.73	19.34	-1.70	0.02	0.00	56(55)
	OA	24.85	19.87	20.78	0.00	0.00	0.00	0
Hydrostatic	M	17.62	16.38	15.02	0.00	1.17	0.00	0
	T	38.00	38.00	18.22	0.00	0.00	0.00	0
	P-O1	19.74	19.56	16.90	0.00	0.00	0.00	63(62)
	P-O2	18.74	18.59	16.09	-0.71	0.00	0.00	64(64)
	OA	17.63	20.49	17.31	0.00	0.00	0.00	0
Equibiaxial ($\epsilon=4.3\%$)	M	18.47	16.48	15.49	0.00	0.80	0.00	0
	T	67.39	67.39	16.97	0.00	0.00	0.00	0
	P-O1	21.85	21.87	19.73	0.00	0.00	0.00	55(53)
	P-O2	21.44	21.35	17.88	-0.07	0.00	0.00	51(49)
	OA	22.30	18.78	20.15	0.00	0.00	0.00	0