Towards an accurate description of perovskite ferroelectrics: exchange and correlation effects

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Supplementary Information

The detailed structural information on each crystal phase of $PbTiO_3$, $BaTiO_3$, and $KNbO_3$ is summarized in Table S1, using LDA, PBE, PBEsol, and vdW-DF-C09 exchange-correlation functionals.

Table S1. Structural information (Wyckoff positions of atoms in fractional coordinates with respect to unit cells) of different crystal phases of $PbTiO_3$, $BaTiO_3$, and $KNbO_3$, using LDA, PBE, PBEsol, and vdW-DF-C09.

Cubic Phase (Pm-3m)

$PbTiO_3$:

	LDA	**PBE**	**PBEsol**	**vdW-DF-C09**	**Experiment[1]**
a (Å)	3.881	3.966	3.919	3.921	3.930

$BaTiO_3$:

	LDA	**PBE**	**PBEsol**	**vdW-DF-C09**	**Experiment[2]**
a (Å)	3.941	4.026	3.977	3.981	4.000

$KNbO_3$:

	LDA	**PBE**	**PBEsol**	**vdW-DF-C09**	**Experiment[3]**
a (Å)	3.952	4.025	3.986	3.988	4.005

Tetragonal Phase (P4mm)

$PbTiO_3$:

	LDA	**PBE**	**PBEsol**	**vdW-DF-C09**	**Experiment[4]**
a (Å)	3.858	3.837	3.865	3.895	3.904
c (Å)	4.017	4.787	4.228	4.076	4.152
Atom	Δz_{atom}	Δz_{atom}	Δz_{atom}	Δz_{atom}	Δz_{atom}
Pb: 1a (0, 0, 0)	---	---	---	---	---
Ti: 1b (0.5, 0.5, 0.5+Δz_{Ti})	0.033	0.056	0.040	0.031	0.0400
O_1: 1b (0.5, 0.5, Δz_{O1})	0.088	0.195	0.122	0.090	0.1120
O_2: 2c (0, 0.5, 0.5+Δz_{O2})	0.100	0.171	0.126	0.100	0.1120

$BaTiO_3$:

	LDA	**PBE**	**PBEsol**	**vdW-DF-C09**	**Experiment[5]**
a (Å)	3.933	3.991	3.962	3.969	3.992
c (Å)	3.980	4.216	4.059	4.039	4.036
Atom	Δz_{atom}	Δz_{atom}	Δz_{atom}	Δz_{atom}	Δz_{atom}
Ba: 1a (0, 0, 0)	---	---	---	---	---
Ti: 1b (0.5, 0.5, 0.5+Δz_{Ti})	0.013	0.018	0.016	0.016	0.0203
O_1: 1b (0.5, 0.5, Δz_{O1})	-0.021	-0.052	-0.031	-0.025	-0.0259
O_2: 2c (0, 0.5, 0.5+Δz_{O2})	-0.013	-0.03	-0.019	-0.015	-0.0123

$KNbO_3$:

	LDA	**PBE**	**PBEsol**	**vdW-DF-C09**	**Experiment[3]**
a (Å)	3.944	3.994	3.969	3.975	3.997
c (Å)	3.984	4.205	4.061	4.048	4.063
Atom	Δz_{atom}	Δz_{atom}	Δz_{atom}	Δz_{atom}	Δz_{atom}
K: 1a (0, 0, 0)	---	---	---	---	---
Nb: 1b (0.5, 0.5, 0.5+Δz_{Nb})	0.010	0.018	0.015	0.015	0.0230
O_1: 1b (0.5, 0.5, Δz_{O1})	-0.017	-0.045	-0.027	-0.022	-0.0170
O_2: 2c (0, 0.5, 0.5+Δz_{O2})	-0.018	-0.033	-0.024	-0.021	-0.0190

Orthorhombic Phase (Amm2)

$BaTiO_3$:

	LDA	PBE	PBEsol	vdW-DF-C09	Experiment[6]
a (Å)	3.931	3.977	3.956	3.964	3.990
b (Å)	5.599	5.796	5.675	5.665	5.669
c (Å)	5.609	5.848	5.696	5.681	5.682

Atom	Δy_{atom}	Δz_{atom}	Δy_{atom}	Δz_{atom}	Δy_{atom}	Δz_{atom}	Δy_{atom}	Δz_{atom}	Δy_{atom}	Δz_{atom}
Ba: 2a (0, 0, 0)	---	---	---	---	---	---	---	---	---	---
Ti: 2b (0.5, 0, 0.5+Δz_{Ti})	---	0.011	---	0.017	---	0.014	---	0.013	---	0.010
O_1: 2a (0, 0, 0.5+Δz_{O1})	---	-0.011	---	-0.023	---	-0.016	---	-0.013	---	-0.010
O_2: 4e (0.5, 0.25-Δy_{O1}, 0.75+Δz_{O2})	0.003	-0.013	0.009	-0.026	0.005	-0.018	0.004	-0.015	0.003	-0.013

$KNbO_3$:

	LDA	PBE	PBEsol	vdW-DF-C09	Experiment[3]
a (Å)	3.941	3.984	3.963	3.970	3.973
b (Å)	5.610	5.788	5.682	5.677	5.695
c (Å)	5.616	5.822	5.699	5.691	5.721

Atom	Δy_{atom}	Δz_{atom}	Δy_{atom}	Δz_{atom}	Δy_{atom}	Δz_{atom}	Δy_{atom}	Δz_{atom}	Δy_{atom}	Δz_{atom}
K: 2a (0, 0, 0)	---	---	---	---	---	---	---	---	---	---
Nb: 2b (0.5, 0, 0.5+Δz_{Nb})	---	-0.008	---	-0.016	---	-0.012	---	-0.012	---	-0.017
O_1: 2a (0, 0, 0.5+Δz_{O1})	---	0.016	---	0.026	---	0.020	---	0.018	---	0.004
O_2: 4e (0.5, 0.25-Δy_{O1}, 0.75+Δz_{O2})	0	0.013	-0.006	0.024	-0.002	0.018	-0.001	0.016	-0.013	0.018

Rhombohedral Phase (R3m)

$BaTiO_3$:

	LDA	PBE	PBEsol	vdW-DF-C09	Experiment[7]
a (Å)	3.951	4.068	3.998	3.951	4.000

Atom	Δx_{atom}	Δz_{atom}	Δx_{atom}	Δz_{atom}	Δx_{atom}	Δz_{atom}	Δx_{atom}	Δz_{atom}	Δx_{atom}	Δz_{atom}
Ba: 1a (0, 0, 0)	---	---	---	---	---	---	---	---	---	---
Ti: 1a (0.5+Δx_{Ti}, 0.5+Δx_{Ti}, 0.5+Δx_{Ti})	-0.009	-0.009	-0.015	-0.015	-0.012	-0.012	-0.011	-0.011	-0.013	-0.013
O_1: 3b (0.5+Δx_{O1}, 0.5+Δx_{O1}, Δz_{O1})	0.009	0.014	0.016	0.027	0.012	0.019	0.010	0.016	0.011	0.019

$KNbO_3$:

	LDA	PBE	PBEsol	vdW-DF-C09	Experiment[3]
a (Å)	3.959	4.061	4.002	3.959	4.016

Atom	Δx_{atom}	Δz_{atom}	Δx_{atom}	Δz_{atom}	Δx_{atom}	Δz_{atom}	Δx_{atom}	Δz_{atom}	Δx_{atom}	Δz_{atom}
K: 1a (0, 0, 0)	---	---	---	---	---	---	---	---	---	---
Nb: 1a (0.5+Δx_{Nb}, 0.5+Δx_{Nb}, 0.5+Δx_{Nb})	-0.007	-0.007	-0.013	-0.013	-0.011	-0.011	-0.010	-0.010	-0.011	-0.011
O_1: 3b (0.5+Δx_{O1}, 0.5+Δx_{O1}, Δz_{O1})	0.012	0.010	0.017	0.022	0.014	0.016	0.013	0.013	0.018	0.020

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