LATTICE DYNAMICS CALCULATION OF THE IONIC CRYSTALS WITH ION DIPOLE AND QUADRUPOLE DEFORMATIONS: PEROVSKITE STRUCTURE OXIDES

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The Gordon-Kim electron gas model is generalized to include dipole and quadrupole polarizations of the ions. The expression for total energy and dynamical matrix of ionic crystals is derived. The phonons dispersion, dielectric constants, Born effective charges for cubic perovskite structure oxides are calculated and are compared with previous LDA results. Some results of the present calculations are shown in Tables.

Table 1. Calculated lattice parameters (a_0),dielectric constants(ε_∞), quadrupole moments (q_{zz}), Born effective charges (Z^*) for ABO_3 perovskites.

crystal	$a_{0,}$ Ă	ε_∞	q_{zz}	$Z^*(A)$	$Z^*(B)$	$Z^*_\perp(O)$	$Z^*_{\|\|}(O)$
$BaTiO_3$	3.86	4.95	0.93	2.98	5.98	-1.68	-5.60
$SrTiO_3$	3.78	4.18	0.81	2.61	5.78	-1.67	-5.05
$PbTiO_3$	3.84	4.79	0.79	2.83	5.69	-1.72	-5.07
$CaTiO_3$	3.73	4.37	0.82	2.66	6.00	-1.77	-5.12
$PbZrO_3$	4.02	4.56	0.87	2.85	5.58	-1.97	-4.48
$BaZrO_3$	4.05	4.41	0.94	2.88	5.61	-1.95	-4.60
$NaNbO_3$	3.76	3.50	1.48	1.16	6.91	-1.33	-5.42
$KNbO_3$	3.78	3.72	1.48	1.25	6.89	-1.36	-5.41
$KTaO_3$	3.94	2.79	1.37	1.16	4.61	-1.68	-2.41

Table 2. Calculated optical phonon frequencies (cm^{-1}) for ABO_3 perovskites. Imaginary frequencies indicate soft mode.

crystal	TO1	TO2	TO3	T_{2u}	LO1	LO2	LO3
$BaTiO_3$	58i	226	413	199	155	327	610
$SrTiO_3$	26	260	501	199	168	350	695
$PbTiO_3$	83i	232	422	190	141	325	600
$CaTiO_3$	101i	284	567	175	184	359	755
$PbZrO_3$	86i	215	485	157	107	285	607
$BaZrO_3$	63i	223	474	168	119	298	604
$NaNbO_3$	55i	239	603	161	154	313	816
$KNbO_3$	101	184	554	185	184	303	762
$KTaO_3$	113	251	700	213	155	346	744