Supplementary Materials for

Ternary multicomponent Ba/Mg/Si compounds with inherent bonding hierarchy and rattling Ba atoms toward low lattice thermal conductivity

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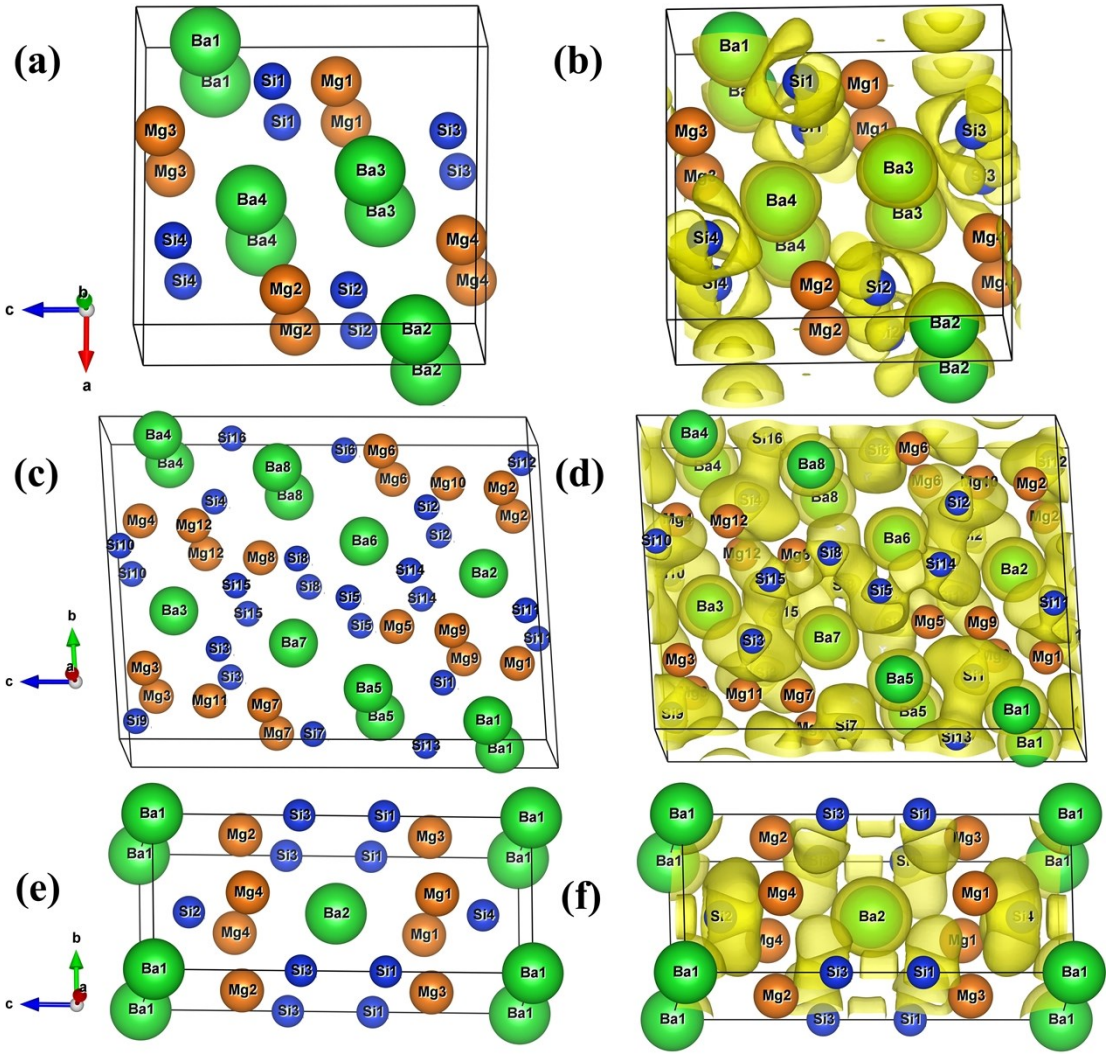

Figure S1: The crystal structures, electron localization function (ELF) plots of the three-dimensional (3D) for (a and b) BaMgSi, (c and d) $Ba_2Mg_3Si_4$, and (e and f) $BaMg_2Si_2$.

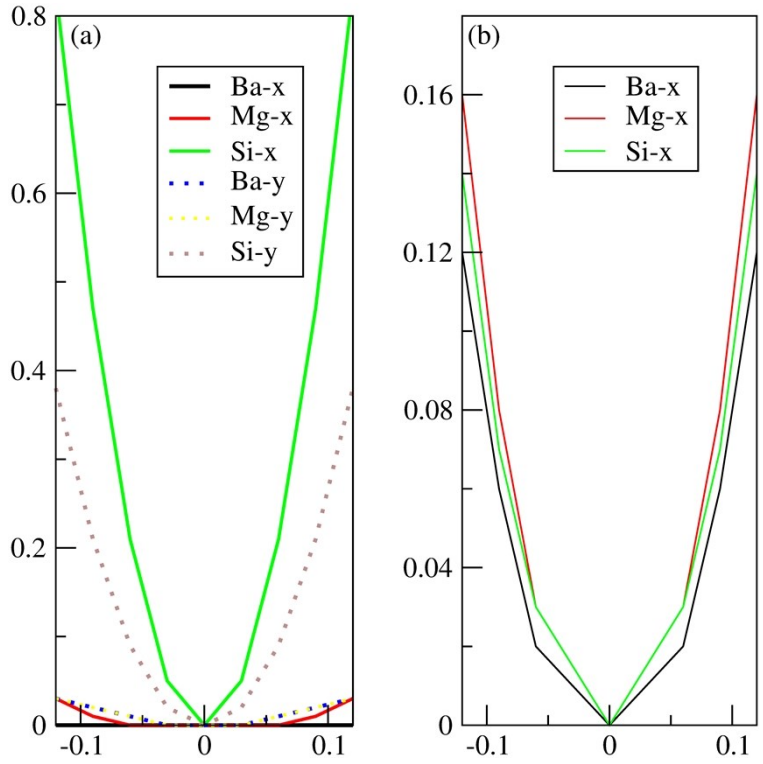

Figure S2: Calculated potential energy surface as a function of displacements of atoms from their equilibrium positions for (a) BaMgSi, and (b) $BaMg_2Si_2$.

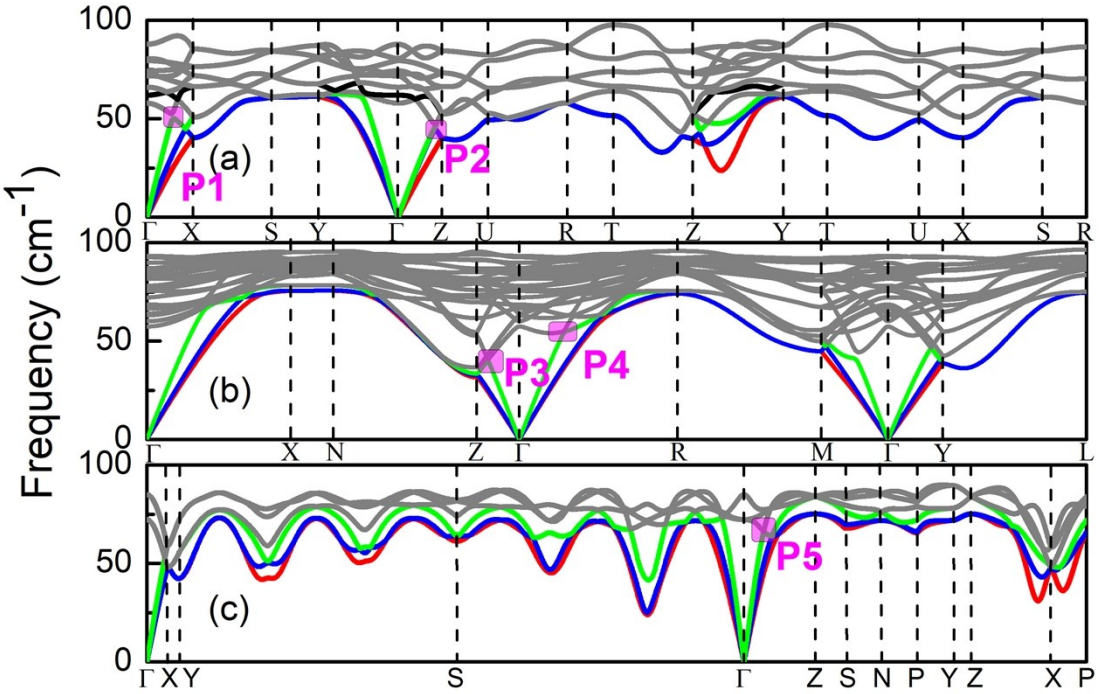

Figure S3: The highlighted phonon dispersion for (a) BaMgSi, (b)$Ba_2Mg_3Si_4$, and (c) $BaMg_2Si_2$.

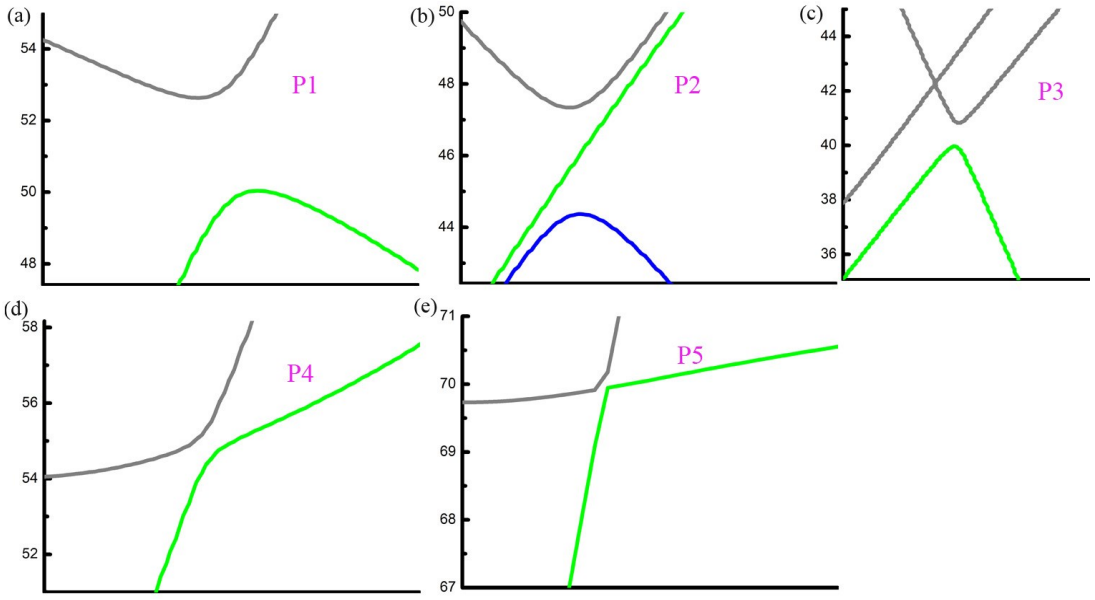

Figure S4: The zoomed-in region for P1-P5 point.

Table S1: The lattice parameters and group spaces for BaMgSi, $Ba_2Mg_3Si_4$, and $BaMg_2Si_2$.

Compounds	Structure	Space group	Lattice parameter (Å)		
			a	b	c
BaMgSi	Orthorhombic	*Pnma*	8.21207	4.77347	8.64639
$Ba_2Mg_3Si_4$	Monoclinic	C_2/m	4.63413	12.14644	15.69401
$BaMg_2Si_2$	Tetragonal	I_4/mmm	4.66514	4.66514	11.04962

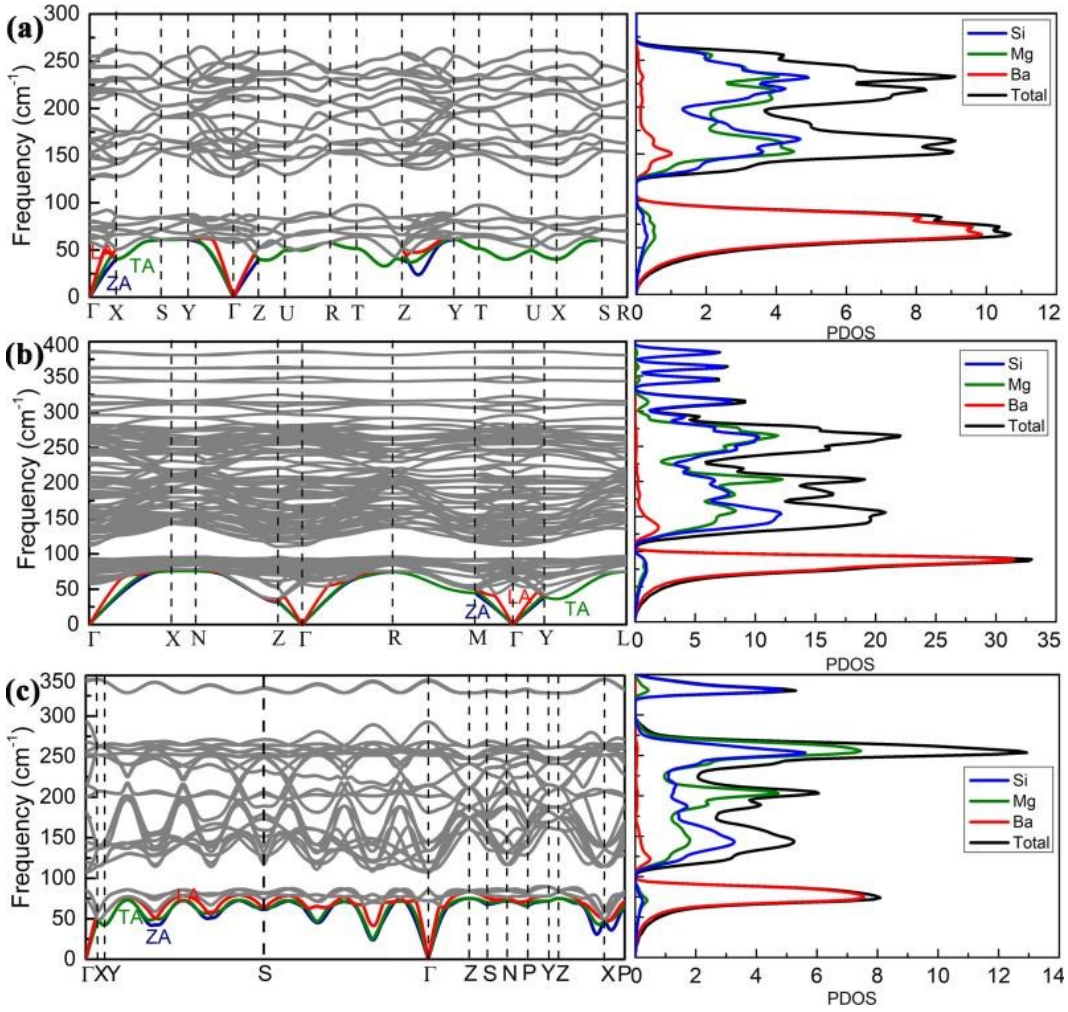

Figure S5: The phonon dispersion for (a) BaMgSi, (b)$Ba_2Mg_3Si_4$, and (c) $BaMg_2Si_2$. Three green, red, blue, and the black lines are TA, LA, ZA acoustic branches, and optical branches, respectively.