Supplemental Material for

‘Predicted crystal structures of xenon and alkali metals under high pressures’

Yifan Tian,[a] John S. Tse,[a,b] Guangtao Liu *[a] and Hanyu Liu[a]

[a]State Key Laboratory of Superhard Materials and International Center for Computational Method & Software, College of Physics, Jilin University, Changchun 130012, China

[b]Physics and Engineering Physics Department, University of Saskatchewan, S7N 5E2, Canada

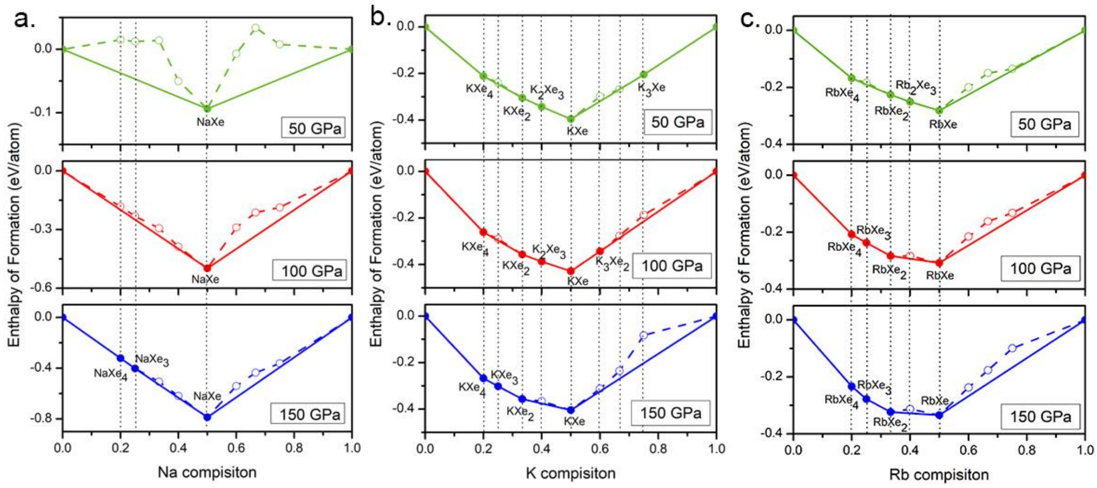

Figure S1. Thermodynamic stabilities of M_xXe_y compounds (M = Na, K and Rb) (a) M = Na, (b) M = K and (c) M = Rb. The solid circles indicate energetically stable phases against decompositions and open circles located above the convex hull indicate the unstable or metastable structures.

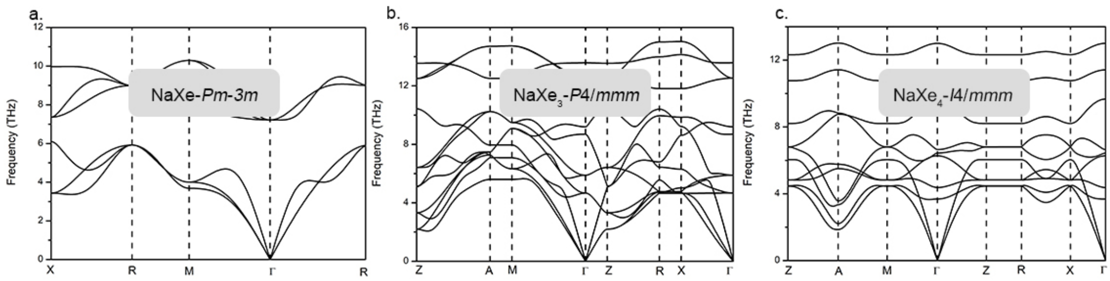

Figure S2. Calculated phonon spectra for various Na–Xe compounds at the respective stable pressure range. (a) NaXe(*Pm*-3*m*) at 30 GPa(b)$NaXe_3$(*P*4/*mmm*) at 150 GPa (c) $NaXe_4$(*I*4/*mmm*) at 150 GPa.

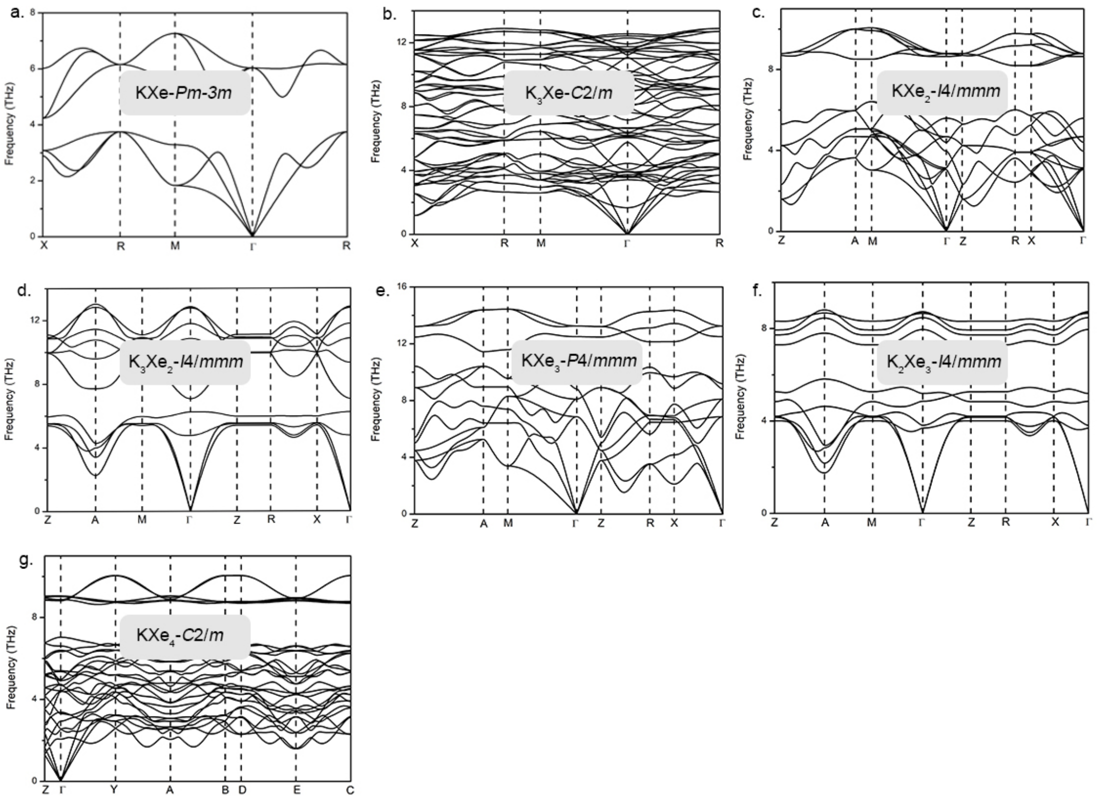

Figure S3. Calculated phonon spectra for various K-Xe compounds at the respective stable pressure range. (a)KXe (*Pm*-3*m*) at 20 GPa (b) K_3Xe (*C*2/*m*) at 50GPa (c) KXe_2 (*I*4/*mmm*) at 50GPa (d) K_3Xe_2(*I*4/*mmm*) at 100 GPa (e) KXe_3 (*P*4/*mmm*) at 150GPa (f) K_2Xe_3 (*I*4/*mmm*) at 50 GPa (g) KXe_4 (*C*2/*m*) at 50 GPa.

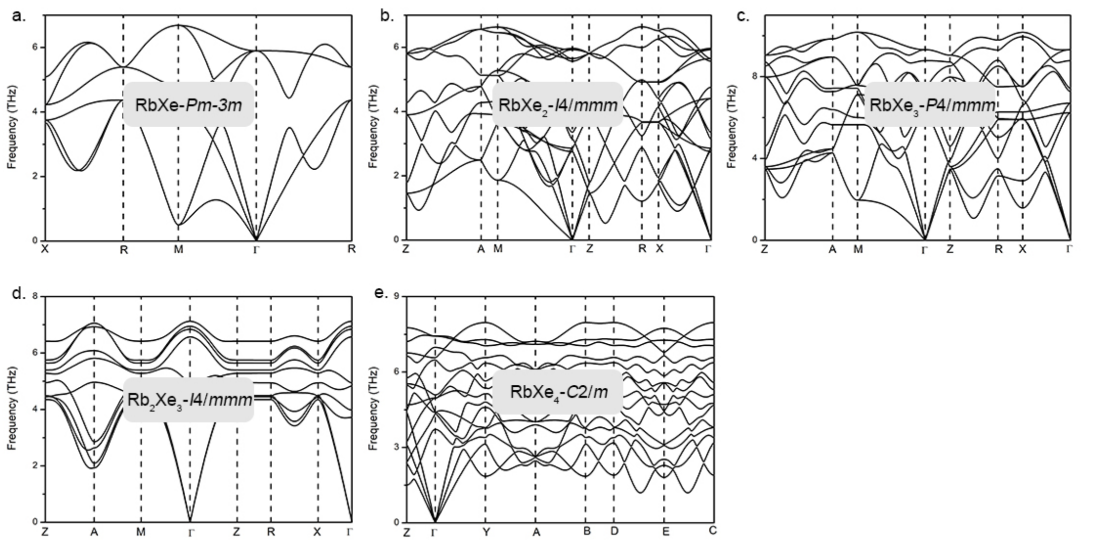

Figure S4. Calculated phonon spectra for various Rb–Xe compounds at the respective stable pressure range. (a)RbXe (*Pm*-3*m*) at 30 GPa(b) $RbXe_2$ (*I*4/*mmm*) at 30GPa (c) $RbXe_3$ (*P*4/*mmm*) at 100GPa (d) Rb_2Xe_3 (*I*4/*mmm*) at 50 GPa (e) $RbXe_4$ (*C*2/*m*) at 50GPa.

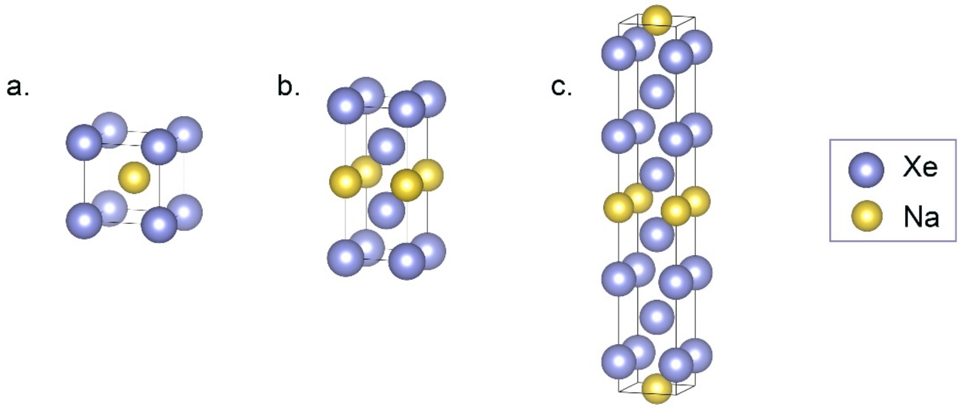

Figure S5. Stable structures of Na–Xe compounds. (a) NaXe (*Pm*-3*m*) (b) $NaXe_3$ (*P*4/*mmm*) (c) $NaXe_4$ (*I*4/*mmm*).

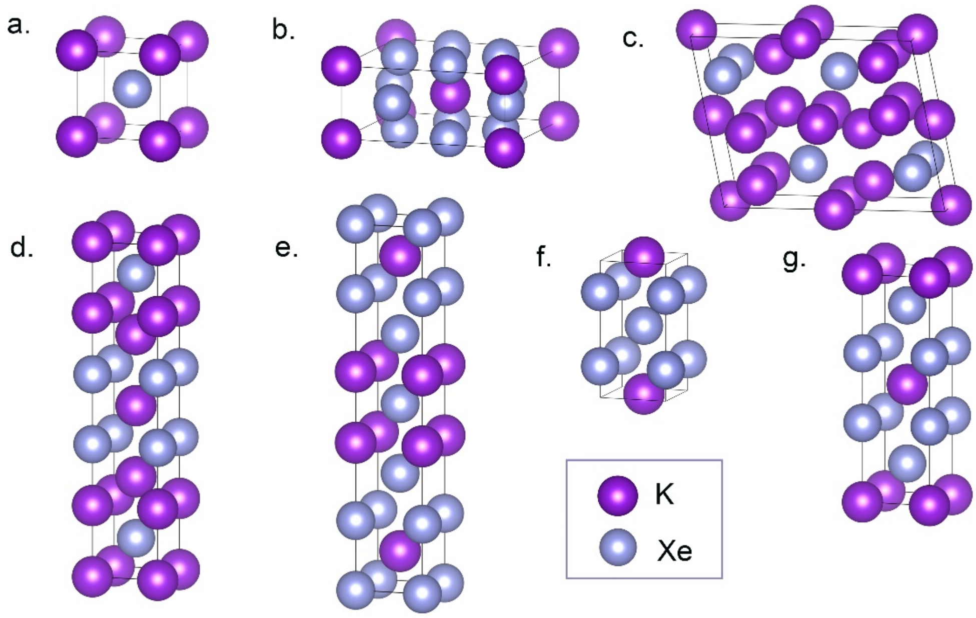

Figure S6. Stable structures of K–Xe compounds. (a) *Pm*-3*m*-KXe (b) *C*2/*m*-KXe_4 (c) *C*2/*m*-K_3Xe (d) *I*4/*mmm*-K_3Xe_2 (e) *I*4/*mmm*-K_2Xe_3 (f) *P*4/*mmm*-KXe_3 (g) *I*4/*mmm*-KXe_2.

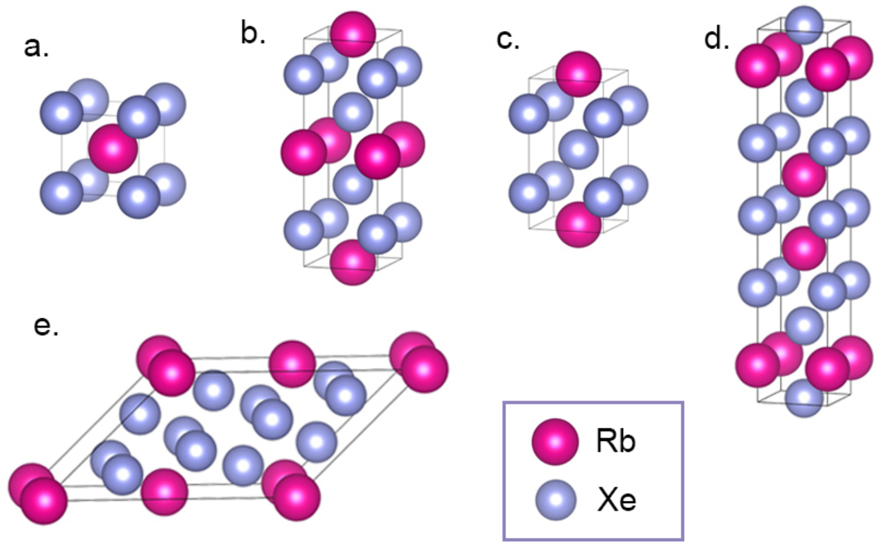

Figure S7. Stable structures of Rb–Xe compounds. (a) *Pm*-3*m*-RbXe (b) *I*4/*mmm*-$RbXe_2$ (c) *P*4/*mmm*-$RbXe_3$ (d) *I*4/*mmm*-Rb_2Xe_3 (e) *C*2/*m*-$RbXe_4$.

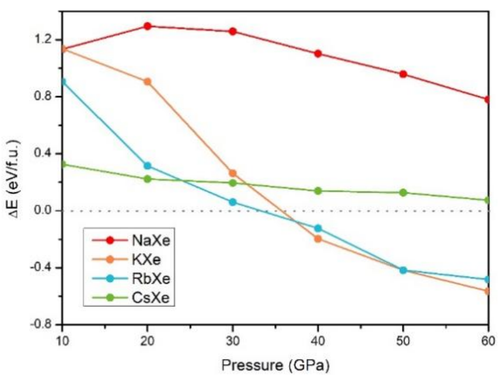

Figure S8. The change of internal energy of compounds NaXe, KXe, RbXe and CsXe versus pressure.

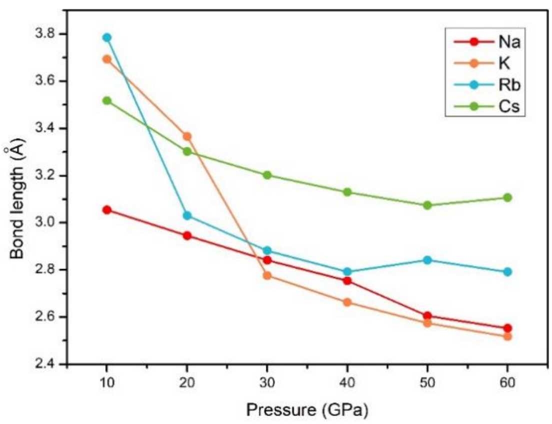

Figure S9. Bond lengths of elements Na, K, Rb and Cs under increasing pressure.

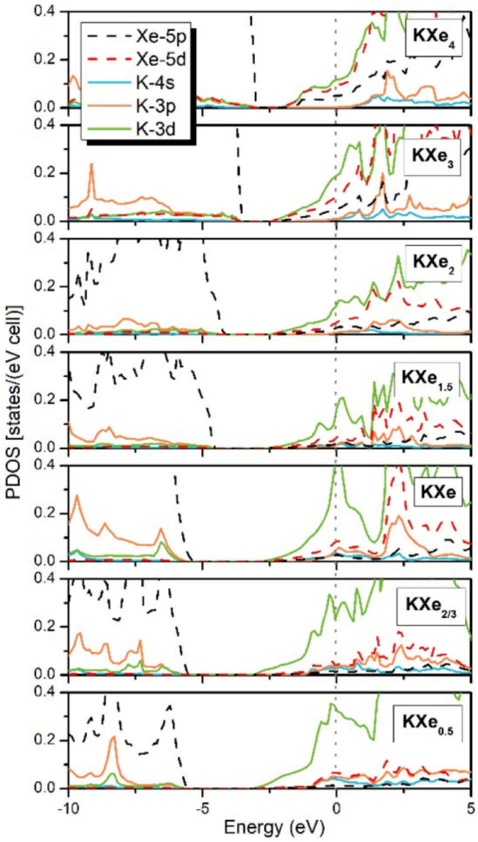

Figure S10. The calculated projected densities of states (PDOS) of various Xe–K compounds at 100 GPa. The vertical dotted line indicates the Fermi energy.

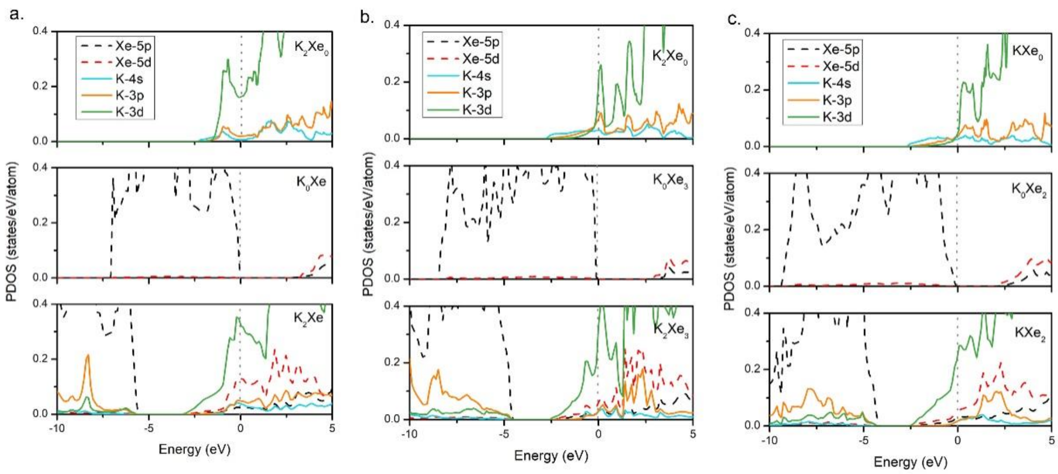

Figure S11. Projected densities of states (PDOS) of different compounds (a) K_2Xe (b) K_2Xe_3 and (c) KXe_2.

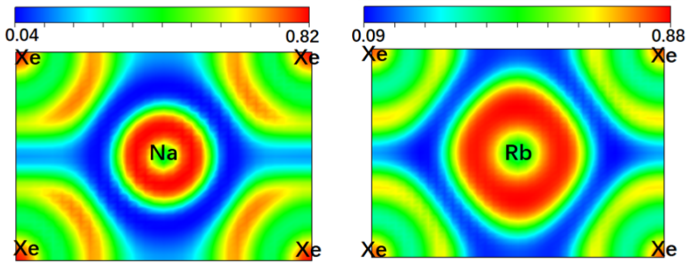

Figure S12. Electron location function (ELF) of the compound NaXe and RbXe (space group *Pm*-3*m*) in the (110) plane at 100 GPa.

Table S1. Crystal Structure Information of Stable Na–Xe, K–Xe and Rb–Xe Compounds

Phases	**P (GPa)**	**lattice parameters (Å, °)**	**atomic coordinates (fractional)**			
NaXe	50	a = b = c = 3.234	Na(1a)	0	0	0
Pm-3m		a = β = γ = 90.0	Xe(1b)	0.5	0.5	0.5
$NaXe_3$	150	a = b = 2.914	Na(1b)	0	0	0.5
P4/mmm		c = 6.950	Xe(2h)	0.5	0.5	0.289
		a = β = γ = 90.0	Xe(1a)	0	0	0
$NaXe_4$	150	a = b = 2.912	Na(2b)	0.5	0.5	0
I4/mmm		c = 17.963	Xe(4e)	0	0	0.306
		a = β = γ = 90.0	Xe(4e)	0.5	0.5	0.418
KXe	50	a = b = c = 3.373	K(1a)	0	0	0
Pm-3m		a = β = γ = 90.0	Xe(1b)	0.5	0.5	0.5
KXe_2	50	a = b = 3.342	K(2b)	0	0	0.5
I4/mmm		c = 11.062	Xe(4e)	0	0	0.847
		a = β = γ = 90.0				
K_2Xe_3	50	a = b = 3.155	K(4e)	0	0	0.097
I4/mmm		c = 16.513	Xe(4e)	0	0	0.310
		a = β = γ = 90.0	Xe(2b)	0.5	0.5	0
K_3Xe	50	a = 10.237	K(4i)	0.165	0	0.560
C2/m		b = 3.464	K(4i)	0.168	0	0.866
		c = 8.029	K(2b)	0	0.5	0
		a = γ = 90	K(2d)	0	0.5	0.5
		β = 79.306	Xe(4i)	0.887	0	0.774
KXe_4	50	a = 11.270	K(4i)	0.25	0	0.25
C2/m		b = 3.429	Xe(4i)	0.151	0	0.566
		c = 11.263	Xe(4i)	0.933	0	0.150
		a = γ = 90	Xe(4i)	0.933	0.5	0.651
		β = 89.971	Xe(4i)	0.151	0.5	0.066
K_3Xe_2	100	a = b = 3.121	K(4e)	0	0	0.212
I4/mmm		c = 15.400	K(2a)	0.5	0.5	0.5
		a = β = γ = 90.0	Xe(4e)	0.5	0.5	0.104
RbXe	50	a = b = c = 3.460	Rb(1a)	0.5	0.5	0.5
Pm-3m		a = β = γ = 90.0	Xe(1b)	0	0	0

$RbXe_2$	50	a = b = 3.489	Rb(2b)	0.5	0.5	0
I*4/*mmm		c = 10.648	Xe(4e)	0	0	0.157
		a = β = γ = 90.0				
Rb_2Xe_3	50	a = b = 3.453	Rb(4e)	0	0	0.902
I*4/*mmm		c = 17.844	Xe(4e)	0	0	0.307
		a = β = γ = 90.0	Xe(2b)	0	0	0.5
$RbXe_3$	100	a = b = 3.347	Rb(1c)	0.5	0.5	0
P*4/*mmm		c = 6.486	Xe(1d)	0.5	0.5	0.5
		a = β = γ = 90.0	Xe(2g)	0	0	0.763
$RbXe_4$	50	a = 11.325	Rb(2a)	0	0	0
C*2/*m		b = 3.495	Xe(4i)	0.411	0	0.199
		c = 8.010	Xe(4i)	0.211	0	0.623
		a = γ = 90				
		β = 134.993				