Supporting information for

Predicted superconductivity in one-dimensional $A_3Hf_2B_3$-type electrides

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Table S1. The structure information and formation energies (E_f) for $Ca_3Hf_2Ge_3$, $Ca_3Hf_2Sn_3$, and $Sr_3Hf_2Pb_3$

Compounds	Space group	Lattice parameters (Å)	E_f (eV/atom)
$Ca_3Hf_2Ge_3$	$P6\bar{3}/mcm$	a = 8.426, c = 6.084	-0.40
$Ca_3Hf_2Sn_3$	$P6\bar{3}/mcm$	a = 8.972, c = 6.187	-0.32
$Sr_3Hf_2Pb_3$	$P6\bar{3}/mcm$	$\boldsymbol{a}$ = 9.454, $\boldsymbol{c}$ = 6.400	-0.05

Table S2. The EPC parameter (λ), ω_{log}, $T_c$for $Ca_3Hf_2Ge_3$, $Ca_3Hf_2Sn_3$, and $Sr_3Hf_2Pb_3$

Compound	Pressure (GPa)	λ	ω_{log} (K)	T_c (K)
$Ca_3Hf_2Ge_3$	0	0.46	139.35	1.16
$Ca_3Hf_2Ge_3$	15	0.54	128.09	1.96
$Ca_3Hf_2Sn_3$	0	0.46	122.63	1.04
$Ca_3Hf_2Sn_3$	12	0.42	138.82	0.71
$Sr_3Hf_2Pb_3$	0	0.74	73.62	4.02
$Sr_3Hf_2Pb_3$	9.3	0.67	101.08	2.69

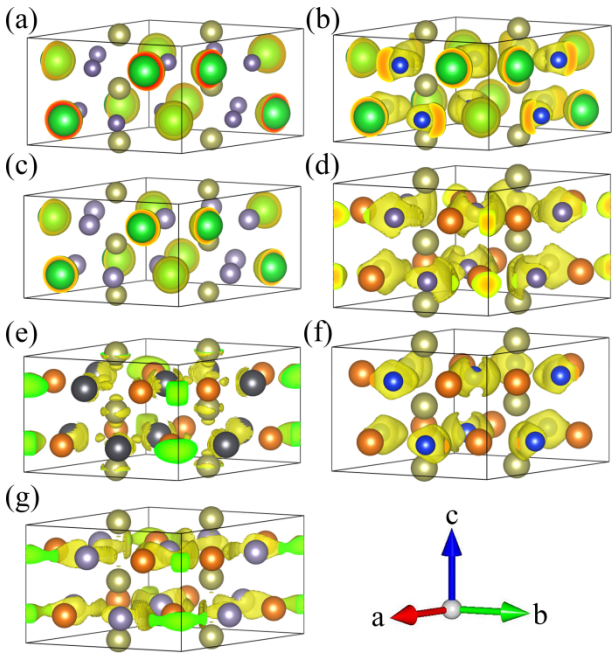

Figure S1. The ELF 3D plots with isosurface value of 0.75 for (a) $Ba_3Hf_2Ge_3$, (b) $Ba_3Hf_2Si_3$, (c) $Ba_3Hf_2Sn_3$, (d) $Mg_3Hf_2Ge_3$, (e) $Mg_3Hf_2Pb_3$, (f) $Mg_3Hf_2Si_3$ and (g) $Mg_3Hf_2Sn_3$. The isosurfaces are plotted at values of 0.75 in (a, b, c, and f), and 0.55 in (d, e, and g), respectively.

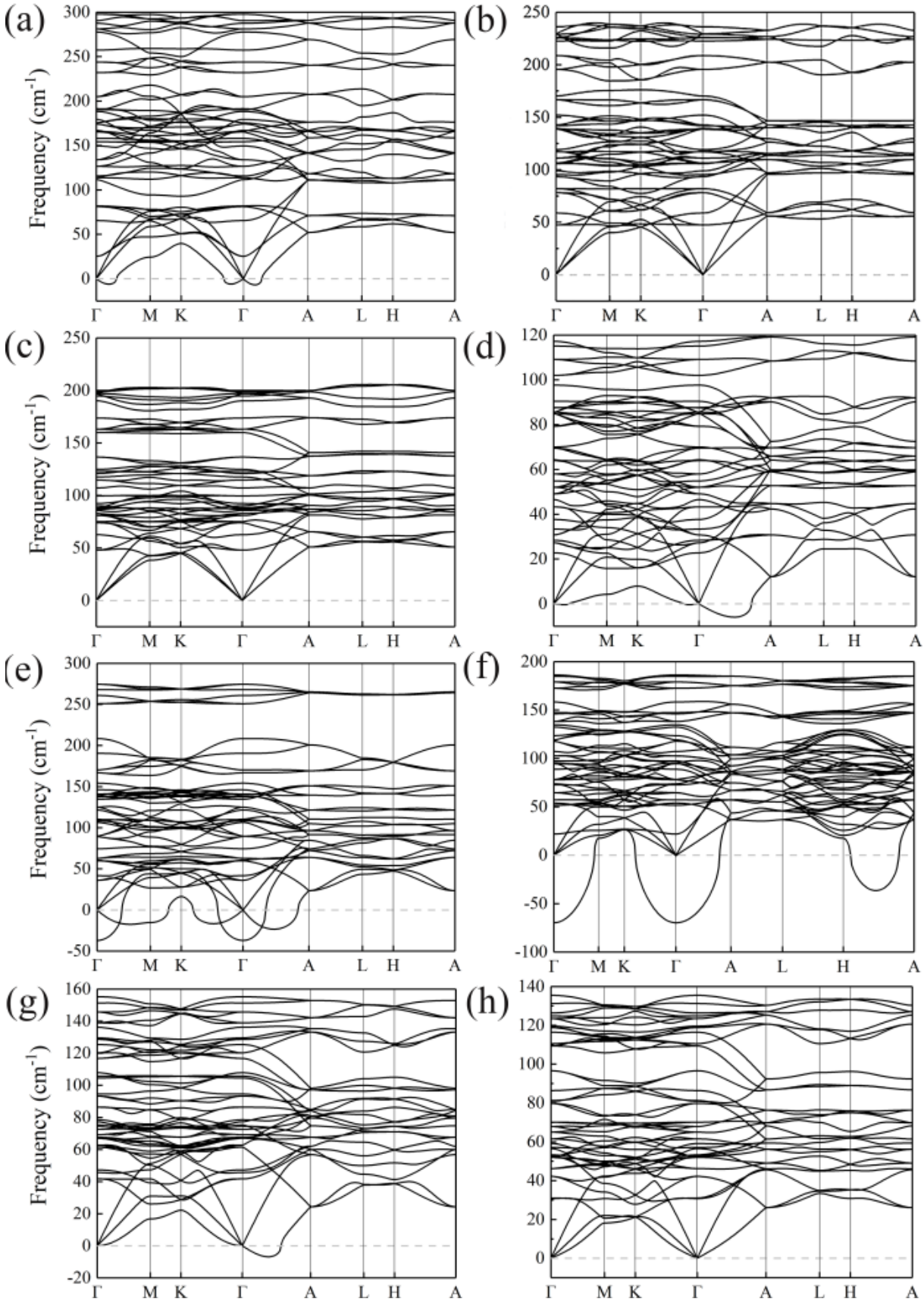

Figure S2. The phonon dispersion curves for (a) $Ca_3Hf_2Si_3$, (b) $Ca_3Hf_2Ge_3$, (c) $Ca_3Hf_2Sn_3$, (d) $Ba_3Hf_2Pb_3$, (e) $Sr_3Hf_2Si_3$, (f) $Sr_3Hf_2Ge_3$, (g) $Sr_3Hf_2Sn_3$ and (h) $Sr_3Hf_2Pb_3$.

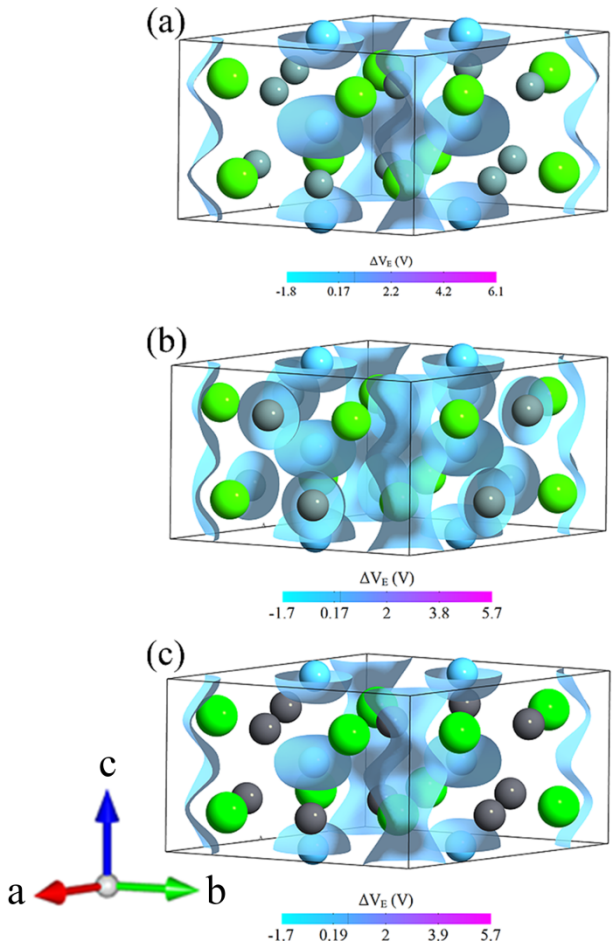

Figure S3**.** The electrostatic difference potential for (a) $Ca_3Hf_2Ge_3$, (b) $Ca_3Hf_2Sn_3$, and (c) $Sr_3Hf_2Pb_3$ with an isosurface value of 0.77 V, 0.38 V, and 0.7 V, respectively.

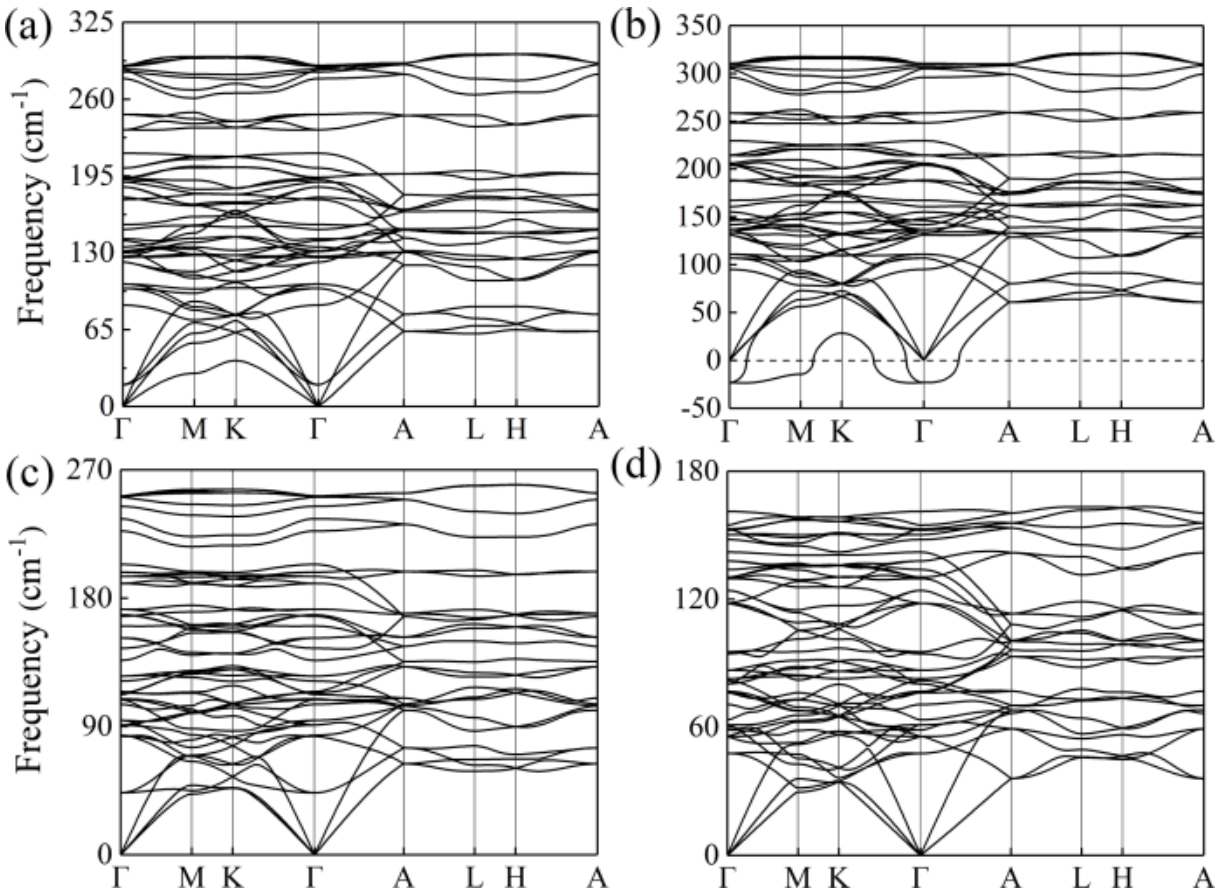

Figure S4. The phonon dispersion curves for $Ca_3Hf_2Ge_3$ at (a) 15 GPa, (b) 20 GPa, (c) $Ca_3Hf_2Sn_3$ at 12 GPa, and (d) $Sr_3Hf_2Pb_3$ at 9.3 GPa.

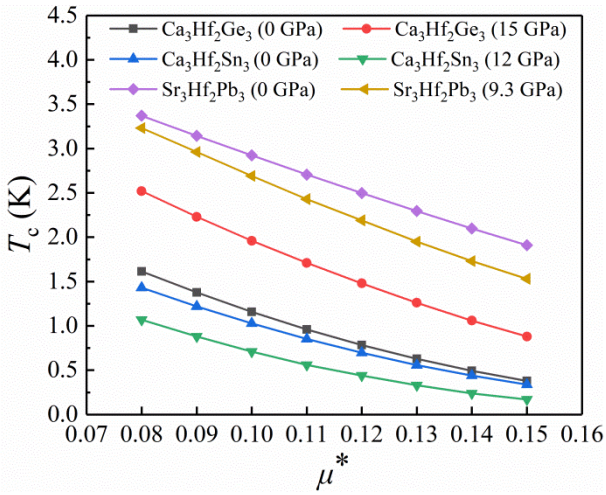

Figure S5. The variation of superconducting transition temperature T_c for $Ca_3Hf_2Ge_3$, $Ca_3Hf_2Sn_3$, $Sr_3Hf_2Pb_3$ with the Coulomb pseudopotential coefficient under different pressures.