SUPPLEMENTARY DOCUMENT

Electronically driven structural transitions in $A_{10}(PO_4)_6F_2$ apatites (A=Ca, Sr, Pb, Cd, and Hg)

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S1.0 DENSITY FUNCTIONAL THEORY

In Table S1, the electronic configurations of the pseudopotentials are given. The input files for the scalar relativistic pseudopotentials were taken from the PSLIBRARY project [1] and the pseudopotentials were generated using the ld1.x routine in the Quantum ESPRESSO package. In our frozen phonon calculations, the atomic displacement amplitudes were set at 0.01Å.

Table S1. Valence electron configurations used in our pseudopotentials.

Element	Valence electron configuration
Ca	$3s^2\ 3p^6\ 4s^2$
Sr	$4s^2\ 4p^6\ 5s^2\ 5p^0$
Pb	$5d^{10}\ 6s^2\ 6p^2$
Cd	$4d^{9.5}\ 5s^2\ 5p^{0.5}$
Hg	$5d^{10}\ 6s^2\ 6p^0$
Zn	$3d^{10}\ 4s^2\ 4p^0$
P	$3s^2\ 3p^3$
O	$2s^2\ 2p^4$
F	$2s^2\ 2p^5$

S2.0 LATTICE DYNAMICAL CALCULATIONS FOR $Zn_{10}(PO_4)_6F_2$

In Figure S1, we show the low-energy zone center phonons for $Zn_{10}(PO_4)_6F_2$ in the aristotype $P6_3/m$ structure. Absence of phonons with negative or imaginary frequencies indicates that the aristotype structure is dynamically stable.

S3.0 CRYSTAL STRUCTURES

The ground state and high symmetry structures are attached separately in *.CIF format.

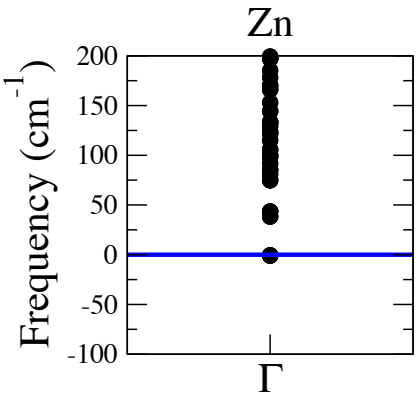

Figure S1 Frequencies (ω) of the low energy zone-center phonons for $Zn_{10}(PO_4)_6F_2$ in the aristotype $P6_3/m$ structure.

REFERENCE

S1. http://qe-forge.org/gf/project/pslibrary/ (v. 0.2.5)