Electronic Supplementary Information (ESI) – Perovskite-type hydrides $ACaH_3$ (A=Li, Na): Computational investigation on materials properties for hydrogen storage applications

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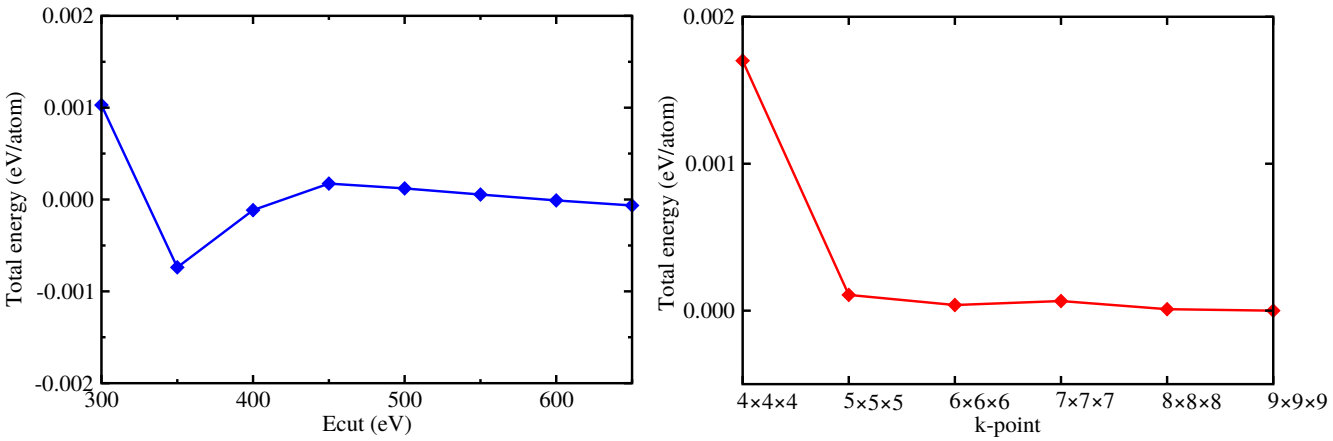

Figure S1 Convergence tests of total energy per atom for a unit cell containing 5 atoms according to the sizes of the energy cutoff and *k*-point mesh for the hydride perovskite $ACaH_3$ (A = Li, Na).

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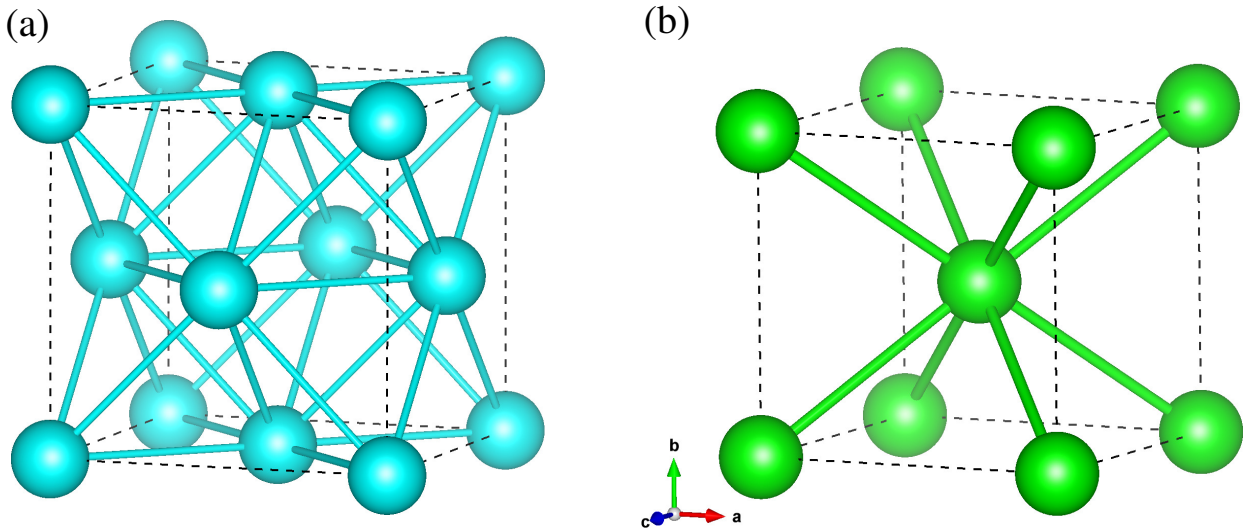

Figure S2 Crystalline structures of (a) the cubic Ca and (b) A compounds with the $Fm\bar{3}m$ and $Im\bar{3}m$ space group, respectively (A = Li, Na).

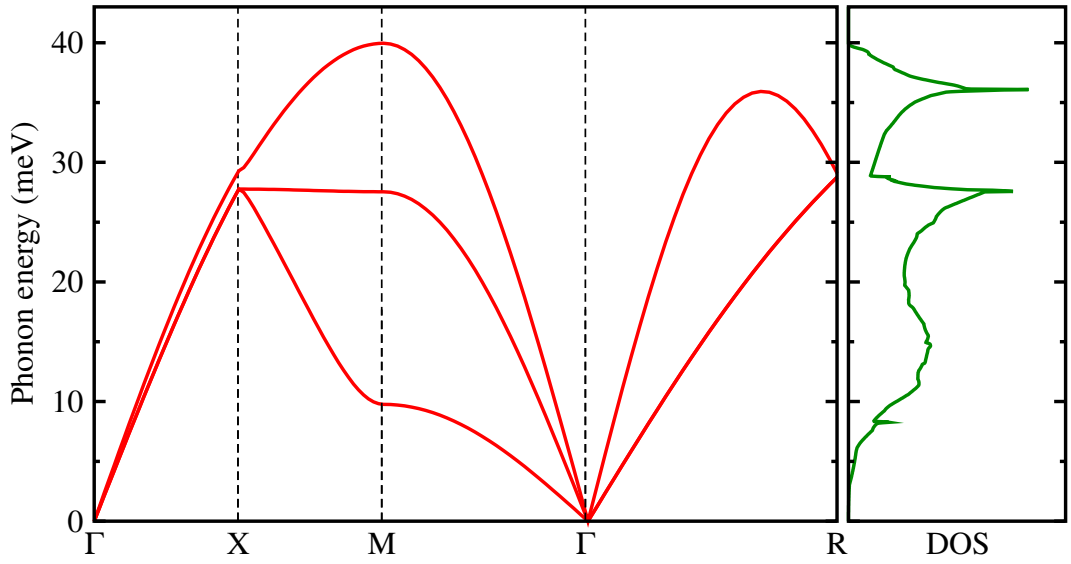

Figure S3 Phonon dispersion curves and phonon density of states (DOS) for the cubic Li with the $Im\bar{3}m$ space group.

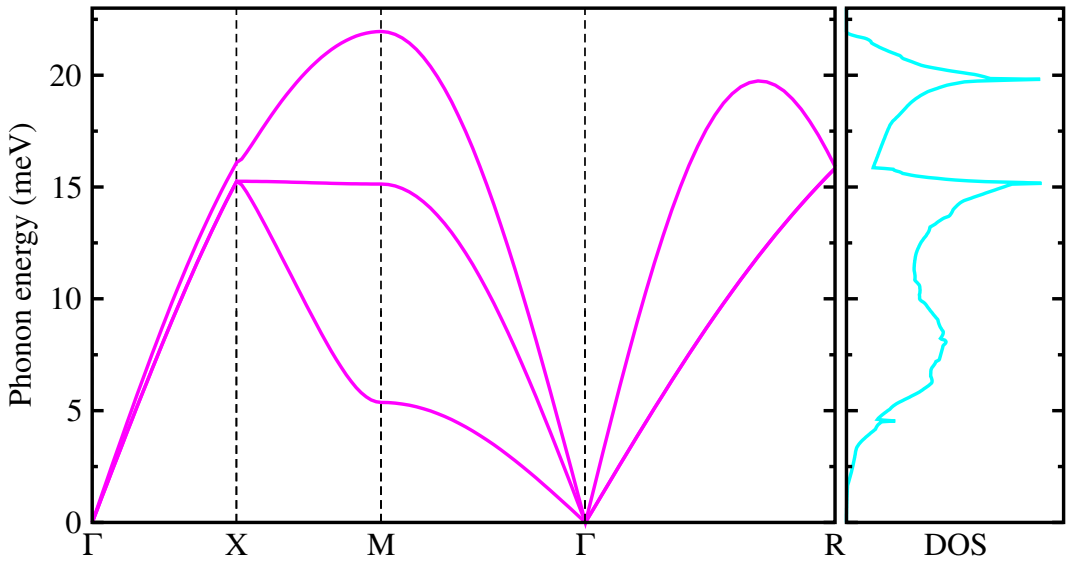

Figure S4 Phonon dispersion curves and phonon density of states (DOS) for the cubic Li with the $Im\bar{3}m$ space group.

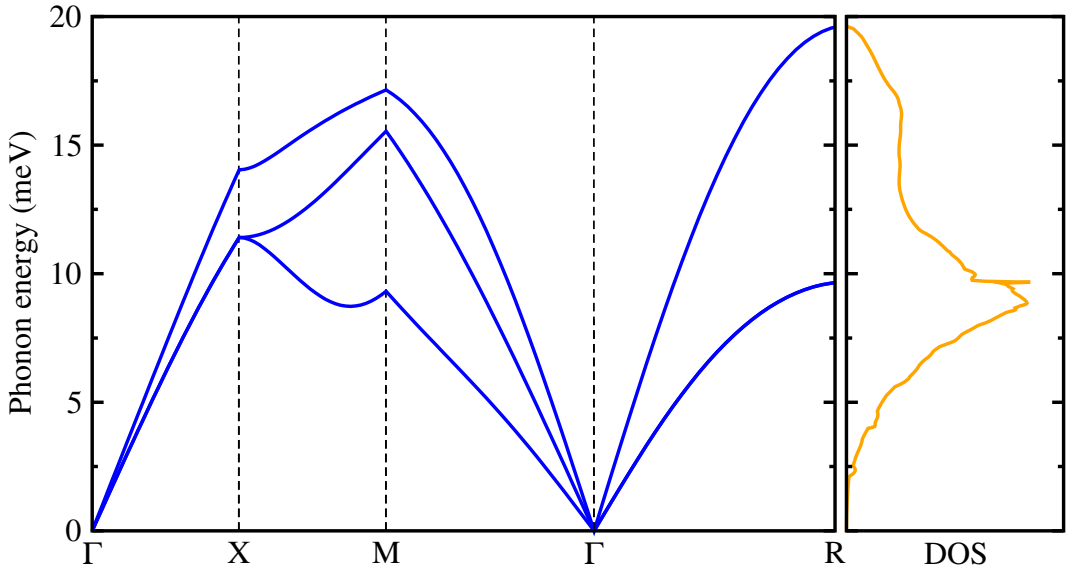

Figure S5 Phonon dispersion curves and phonon density of states (DOS) for the cubic Li with the $Fm\bar{3}m$ space group.

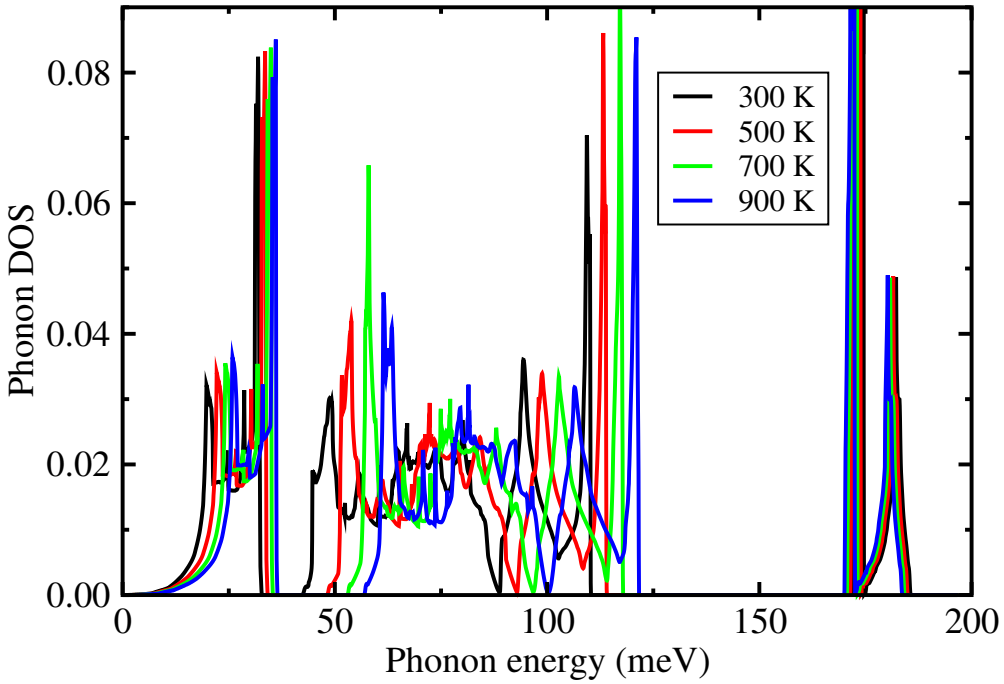

Figure S6 Total phonon density of states (DOS) calculated at 300, 500, 700 and 900 K for the cubic $LiCaH_3$.

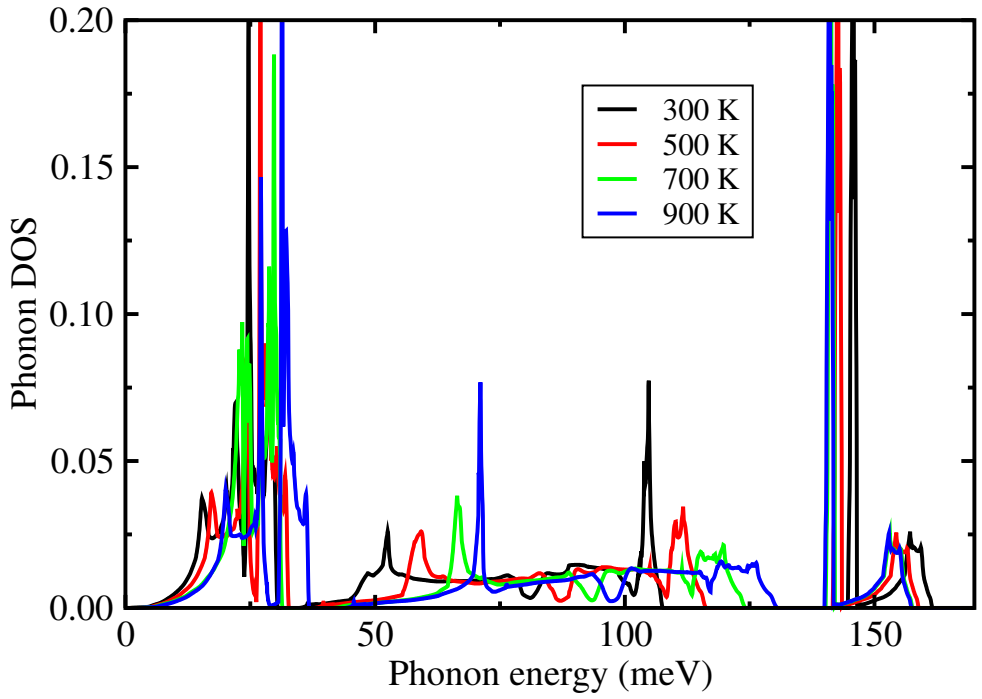

Figure S7 Total phonon density of states (DOS) calculated at 300, 500, 700 and 900 K for the cubic $NaCaH_3$.

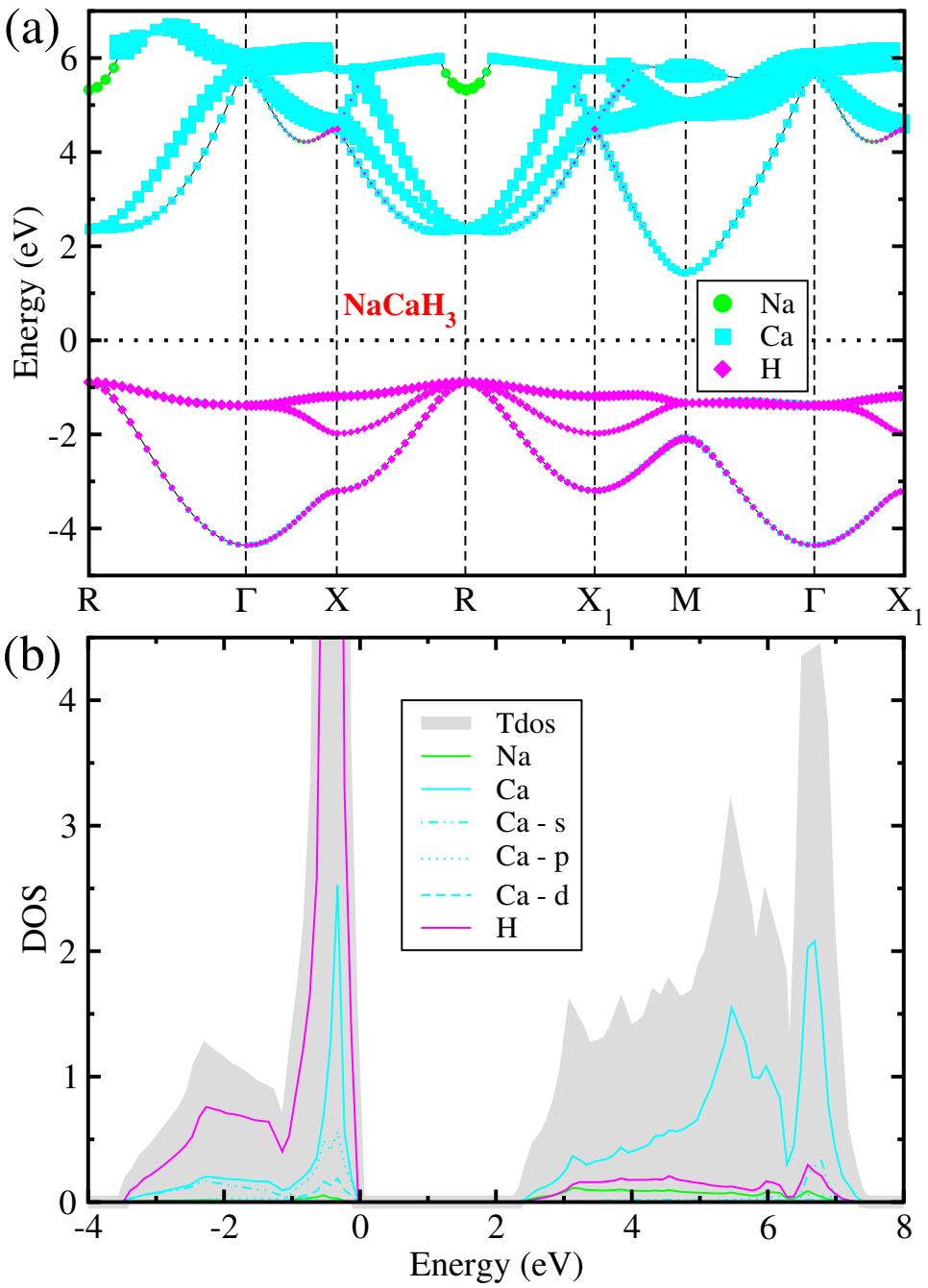

Figure S8 Atom-resolved electronic band structure and (b) partial density of states (DOS) calculated with the PBEsol functional for the hydride perovskite $NaCaH_3$ in the cubic phase.