

Supporting Information

Strain Modulated Hydrogen Storage Aspects, Optoelectronic, and Thermoelectric Energy Harvesting in a Newly Synthesized BaSiH₆

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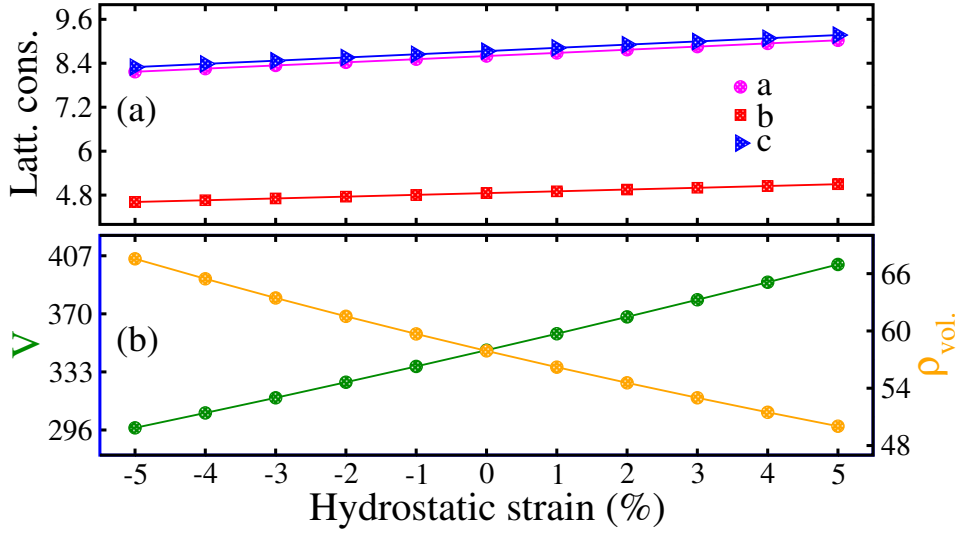


FIG. 1S: Calculated (a) optimized lattice constants (Latt. cons.) in Å, (b-left) unit cell volume (V) in Å³, and (b-right) volumetric capacity ($\rho_{vol.}$) in g.H₂/L as a function of $\pm 5\%$ hydrostatic strain for the BaSiH₆ structure.

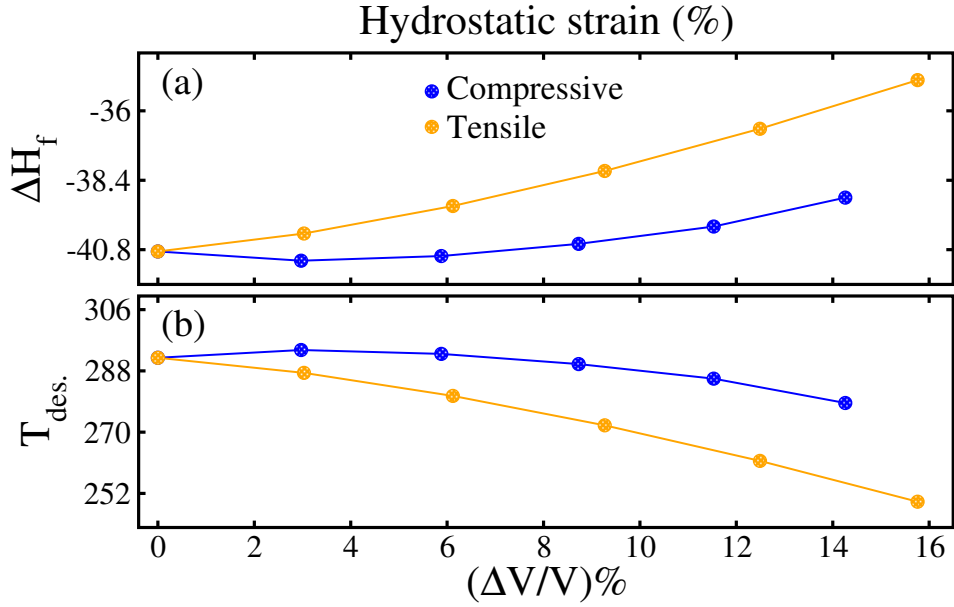


FIG. 2S: Computed (a) formation enthalpy (ΔH) in kJ/mol.H₂ and (b) hydrogen desorption temperature ($T_{des.}$) in K as a function of $\frac{\Delta V}{V}\%$ of the BaSiH₆ structure.

TABLE 1S: Computed numerous elastic properties under hydrostatic-([111]) strain of the BaSiH₆ system.

Strain	Young's modulus			Linear compressibility			Shear modulus			Poisson's ratio	
	Y_{min}	Y_{max}	A	β_{min}	β_{max}	A	G_{min}	G_{max}	A	ν_{min}	ν_{max}
-5%	25.686	101.04	3.93	4.4662	7.2305	1.62	7.32	32.68	4.464	-0.1803	0.86444
0%	18.836	83.86	4.45	5.062	19.698	3.89	8.7775	32.041	3.65	-0.1059	0.83969
+5%	12.883	54.34	4.218	9.348	13.56	1.45	3.63	22.292	6.14	0.05019	0.77489

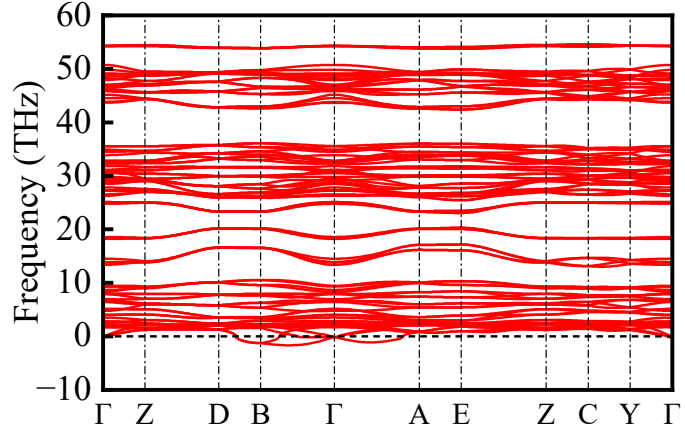


FIG. 3S: Computed phonon dispersion curves of the BaSiH₆ structure.

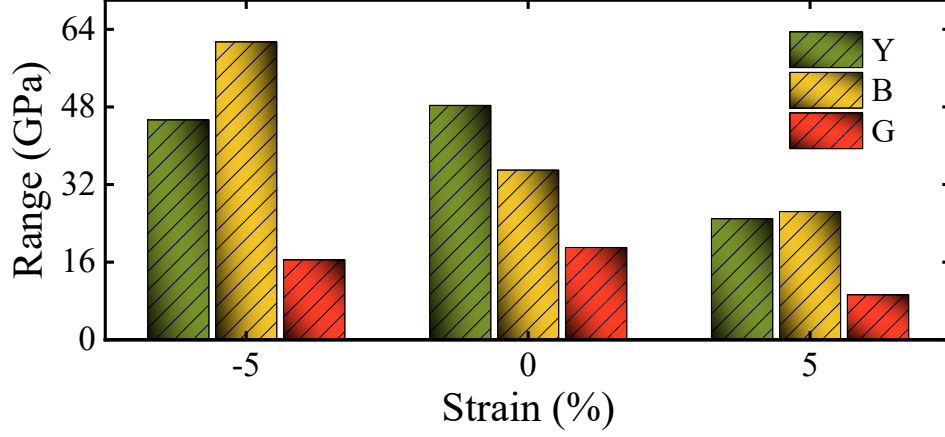


FIG. 4S: Computed bulk modulus (B), Young's modulus (Y), and Shear modulus (G) of the BaSiH₆ structure under -5%/0%/+5% hydrostatic-([111]) strain.

TABLE 2S: Computed numerous elastic properties under hydrostatic-([111]) strain of the BaSiH₆ system.

Strain	Young's modulus			Linear compressibility			Shear modulus			Poisson's ratio		
	Y _{min}	Y _{max}	A	β _{min}	β _{max}	A	G _{min}	G _{max}	A	ν _{min}	ν _{max}	A
-5%	25.686	101.04	3.93	4.4662	7.2305	1.62	7.32	32.68	4.464	-0.1803	0.86444	∞
0%	18.836	83.86	4.45	5.062	19.698	3.89	8.7775	32.041	3.65	-0.1059	0.83969	∞
+5%	12.883	54.34	4.218	9.348	13.56	1.45	3.63	22.292	6.14	0.05019	0.77489	15.4390

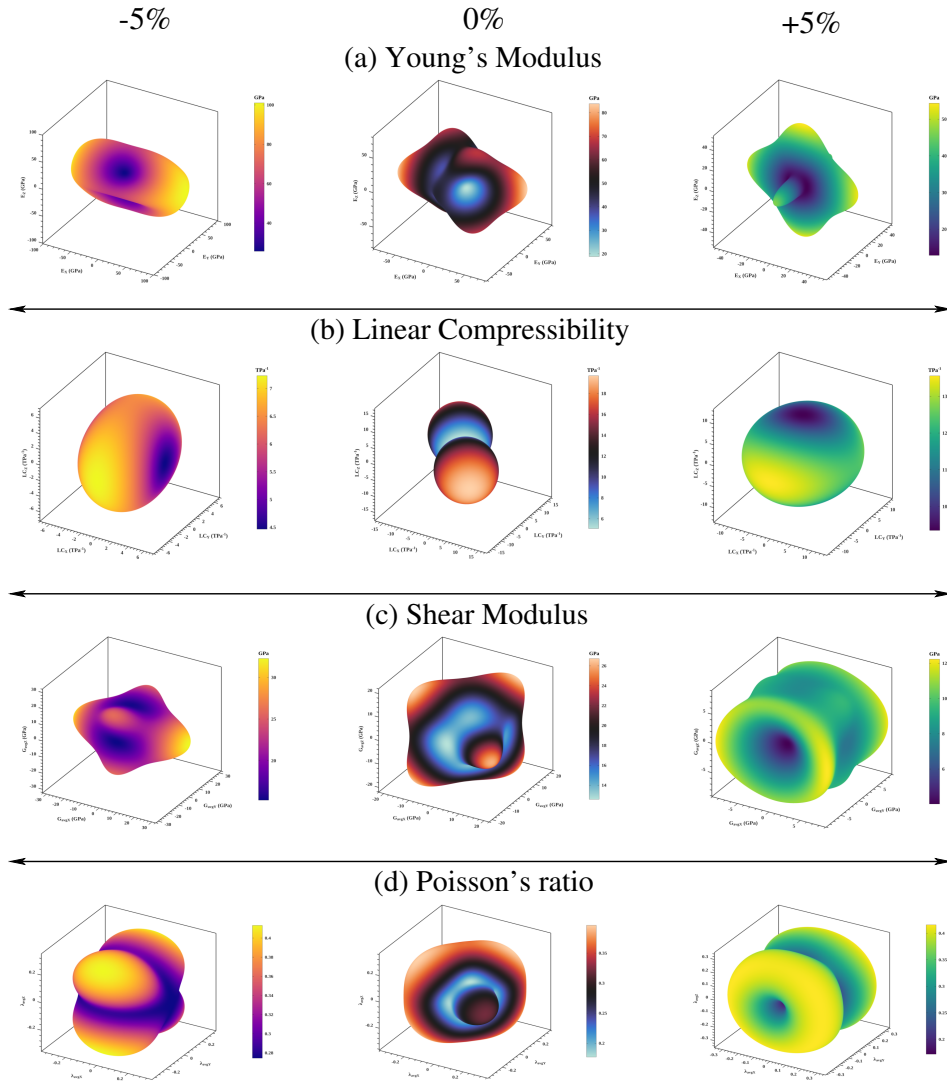


FIG. 5S: Three dimensional directionally dependent (a) Young's modulus, (b) linear compressibility, (c) Shear modulus, and (d) Poisson's ratio for the BaSiH₆ structure under -5% (left column)/ 0% (middle column)/ $+5\%$ (right column) hydrostatic- $([111])$ strain.

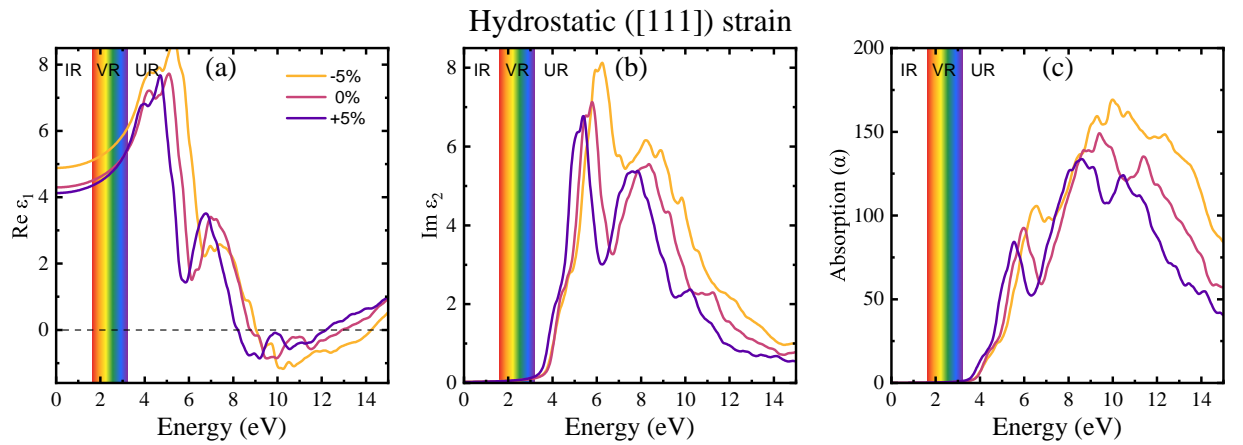


FIG. 6S: Calculated various optical parameters such as (a) real dielectric part ϵ_1 , (b) imaginary dielectric part ϵ_2 , and absorption coefficient (α) in 10^4 cm^{-1} under $-5\%/0\%/+5\%$ hydrostatic $([110])$ strain for the BaSiH₆ structure.

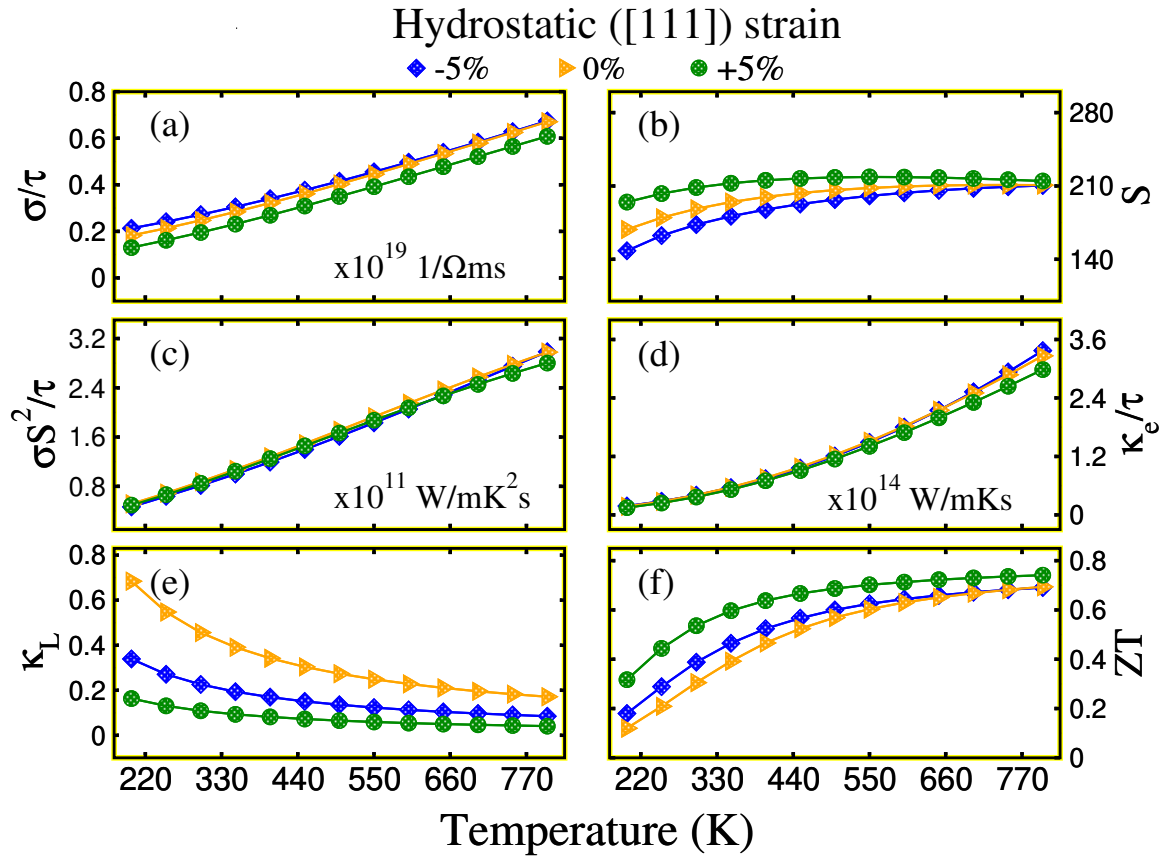


FIG. 7S: Various computed thermoelectric parameters under $-5\%/0\%/+5\%$ hydrostatic-([111]) strain for the BaSiH_6 structure.