

Supplementary information

Predicted stable Li_5P_2 and Li_4P at ambient pressure: novel high performance anodes for lithium-ion batteries

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AFFILIATIONS

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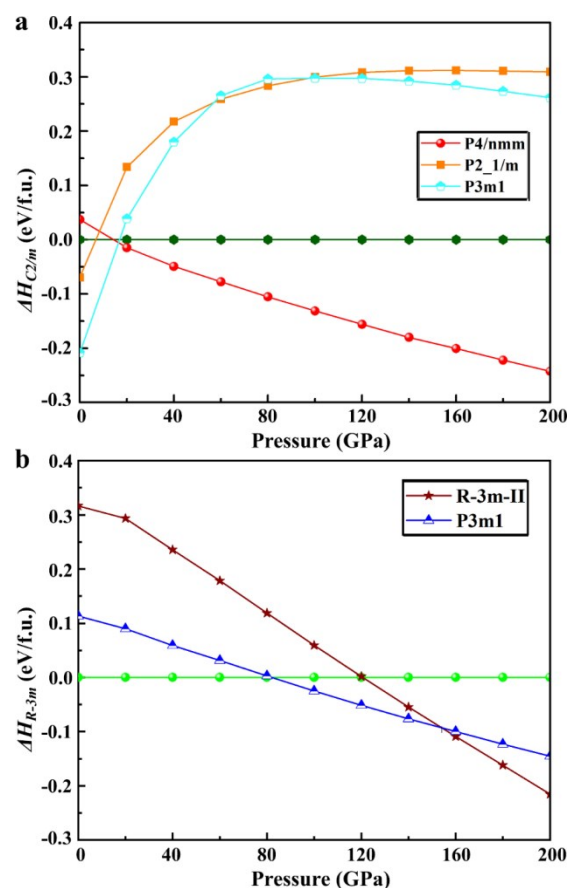


Figure S1. Relative enthalpy per formula unit referenced to C2/m and R-3m phase for Li_5P_2 (top panel) and Li_4P (bottom panel) as a function of pressure from 0 to 200 GPa.

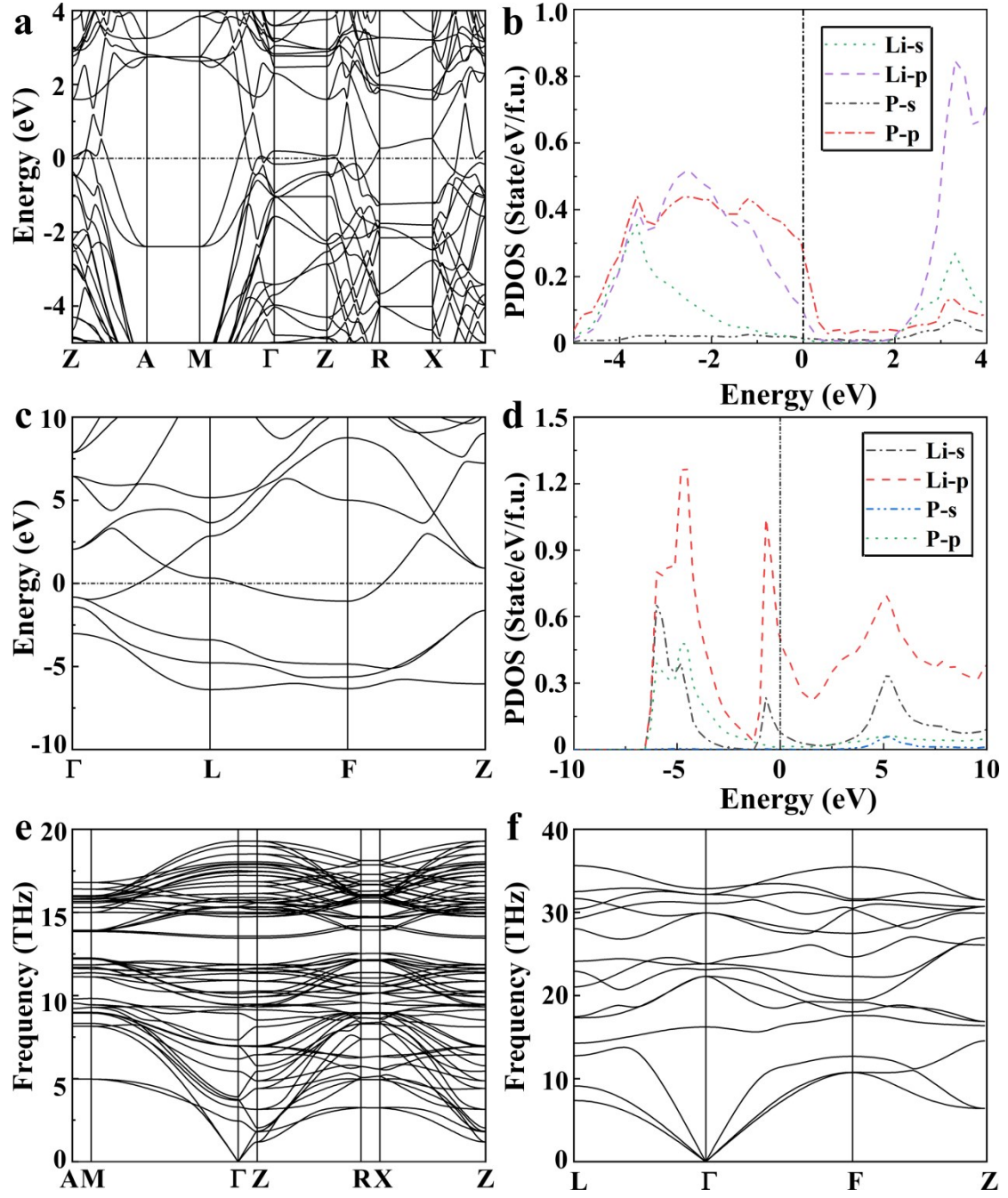


Figure S2. Electronic properties of $P4/nmm$ Li_5P_2 at 200 GPa and $R-3m-II$ Li_4P at 200 GPa. (a) Calculated band structures of $P4/nmm$ Li_5P_2 . (b) PDOS of $P4/nmm$ Li_5P_2 . (c) The calculated phonon spectra of $P4/nmm$ Li_5P_2 . (d) Calculated band structures of $R-3m-II$ Li_4P . (e) PDOS of $R-3m-II$ Li_4P . (f) The calculated phonon spectra of $R-3m-II$ Li_4P .

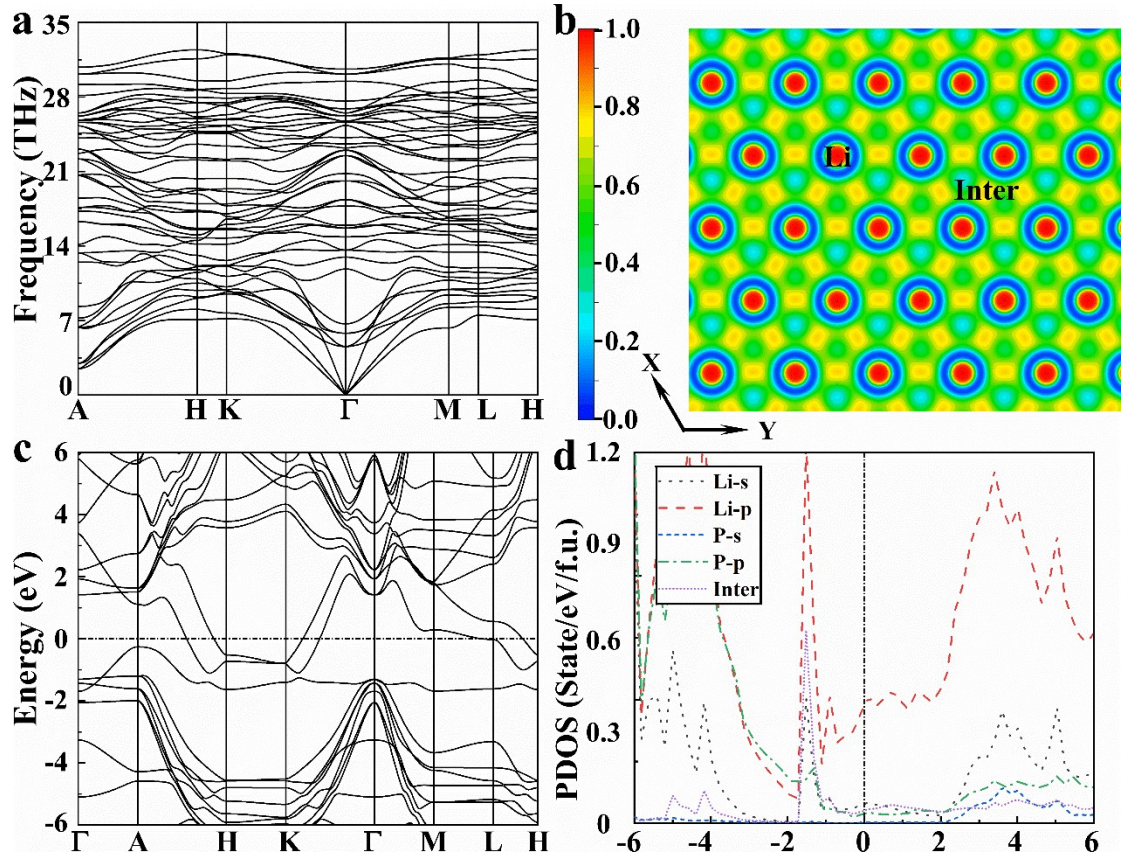


Figure S3. Electronic properties of $P3m1$ Li_4P at 120 GPa. The calculated phonon spectra and the electron localization function (ELF) on the (001) plane are shown in (a) and (b), respectively. (c) Calculated band structure of $P3m1$ Li_4P . (d) Partial density of states (PDOS).

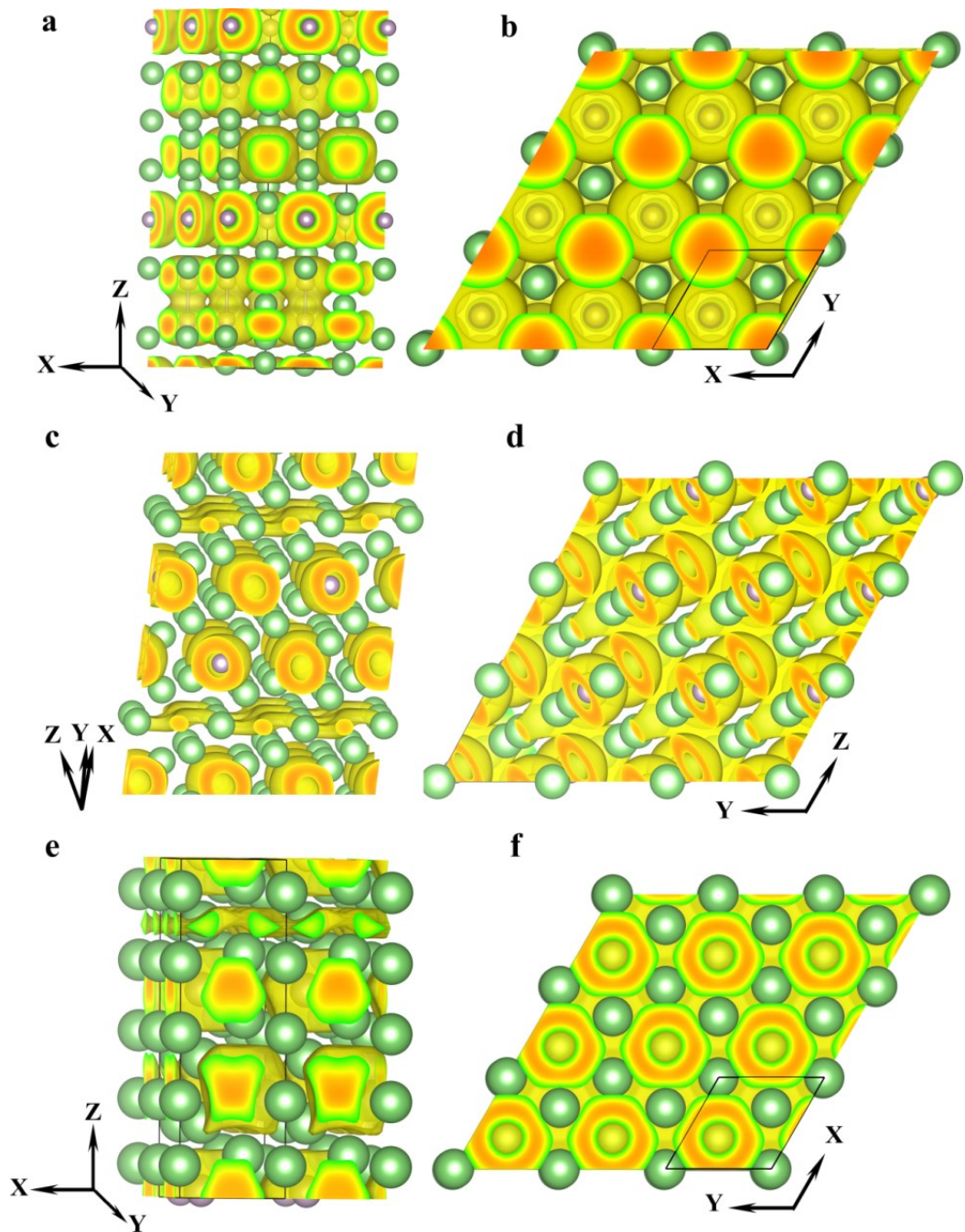


Figure S4. Isosurface of 3D-ELF for Li_5P_2 and Li_4P . (a, b) ELF for $P3m1$ Li_5P_2 plotted with the value of 0.75 at ambient condition. (c, d) ELF for $R-3m$ Li_4P plotted with the value of 0.75 at 0 GPa. (e, f) ELF for $P3m1$ Li_4P with the value of 0.5 at 120 GPa.

Table S1. Structural information of the predicted stable Li-P phases

Phase	Pressure (GPa)	Lattice Parameters (Å, °)	Wyckoff Positions (fractional)			
			Atoms	x	y	z
<i>P3m1</i> Li ₅ P ₂	0	a = b = 4.1921 c = 19.0867 $\alpha = \beta = 90.0$ $\gamma = 120.0$	Li (1a)	-0.00000	1.00000	0.55094
			Li (1a)	-0.00000	1.00000	0.27641
			Li (1a)	-0.00000	1.00000	0.08155
			Li (1c)	0.66667	0.33333	0.64187
			Li (1c)	0.66667	0.33333	0.51106
			Li (1c)	0.66667	0.33333	0.92434
			Li (1c)	0.66667	0.33333	0.37547
			Li (1a)	1.00000	-0.00000	0.68933
			Li (1a)	1.00000	-0.00000	0.82208
			Li (1b)	0.33333	0.66667	0.17386
			Li (1b)	0.33333	0.66667	0.32087
			Li (1b)	0.33333	0.66667	0.73282
			Li (1b)	0.33333	0.66667	0.87419
			Li (1b)	0.33333	0.66667	0.01054
			Li (1b)	0.33333	0.66667	0.45902
			P (1a)	-0.00000	1.00000	0.41266
			P (1c)	0.66667	0.33333	0.24207
			P (1c)	0.66667	0.33333	0.77404
			P (1c)	0.66667	0.33333	0.12510
			P (1a)	1.00000	-0.00000	0.95191
			P (1b)	0.33333	0.66667	0.59326
<i>P4/nmm</i> Li ₅ P ₂	20	a = b = 3.7348	Li (8j)	0.00000	0.50000	0.43102
		c = 20.4602	Li (8j)	0.00000	0.50000	0.70719
		$\alpha = \beta = \gamma = 90.0$	Li (8j)	0.50000	0.50000	0.91892

			Li (8j)	0.50000	0.50000	0.63749
			Li (8j)	0.50000	0.50000	0.22549
			Li (8j)	0.50000	0.00000	0.84317
			Li (4e)	0.00000	0.00000	0.50000
			P (8j)	0.00000	0.50000	0.29441
			P (8j)	0.50000	0.00000	0.99491
			P (8j)	0.50000	0.00000	0.43140
			P (8j)	0.50000	0.00000	0.15721
<i>R-3m</i> Li₄P	0	$a = b = c = 9.3893$ $\alpha = \beta = \gamma = 25.8932$	Li (36i)	-0.59566	-0.59566	-0.59566
			Li (36i)	-0.71371	-0.71371	-0.71371
			Li (36i)	-0.80369	-0.80369	-0.80369
			Li (9d)	-0.50000	-0.50000	-0.50000
			Li (3a)	-0.00000	0.00000	0.00000
			P (36i)	-0.10215	-0.10215	-0.10215
<i>P3m1</i> Li₄P	120	$a = b = 3.3001$ $c = 10.0258$ $\alpha = \beta = 90.0$ $\gamma = 120.0$	Li (1c)	0.66667	0.33333	0.81336
			Li (1c)	0.66667	0.33333	0.22062
			Li (1c)	0.66667	0.33333	0.40993
			Li (1b)	0.33333	0.66667	0.53203
			Li (1b)	0.33333	0.66667	0.12558
			Li (1b)	0.33333	0.66667	0.72070
			Li (1b)	0.33333	0.66667	0.92863
			Li (1a)	-0.00000	0.00000	0.48773
			Li (1a)	-0.00000	0.00000	0.09542
			Li (1a)	-0.00000	0.00000	0.28782
			Li (1a)	-0.00000	0.00000	0.69584
			Li (1a)	-0.00000	0.00000	0.90469
			P (1c)	0.66667	0.33333	0.01566
			P (1c)	0.66667	0.33333	0.61286

			P (1b)	0.33333	0.66667	0.32909
<i>R-3m-II</i> Li₄P	200	$a = b = c = 3.5806$	Li (36i)	0.78816	0.78816	0.78816
		$\alpha = \beta = \gamma = 51.9846$	Li (36i)	0.40551	0.40551	0.40551
			P (3a)	0.00000	-0.00000	-0.00000
