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Pressure effects on the ionic transport properties of $LiNH_2$

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Table S1. Detailed fitting parameters for the mixed ionic and electronic conduction in $LiNH_2$. The CPE_1 and CPE_2 relate to the grain resistance (R_g) and the grain boundary resistance (R_{gb}), respectively.

Pressure (GPa)	CPE1-T	CPE-P	W-T	W-P	R_{gi}	R_{ge}	W_R	CPE2-T	CPE2-P	R_{gb}
0	1.50×10^{-12}	0.890	8.0	0.440	1.30×10^{7}	1.40×10^{8}	1.40×10^{8}	5.80×10^{-11}	0.820	2.00×10^{6}
1.0	1.50×10^{-12}	0.890	11.0	0.445	1.70×10^{7}	1.75×10^{8}	2.15×10^{8}	5.00×10^{-11}	0.800	3.50×10^{6}
1.6	1.50×10^{-12}	0.890	11.0	0.400	1.80×10^{7}	1.80×10^{8}	1.80×10^{8}	5.80×10^{-11}	0.820	4.80×10^{6}
2.1	1.35×10^{-12}	0.895	8.0	0.400	2.15×10^{7}	1.90×10^{8}	2.30×10^{8}	6.20×10^{-11}	0.780	5.50×10^{6}
2.9	1.35×10^{-12}	0.895	9.0	0.420	2.20×10^{7}	1.95×10^{8}	2.25×10^{8}	6.80×10^{-11}	0.780	6.00×10^{6}
3.6	1.35×10^{-12}	0.895	15.0	0.400	2.40×10^{7}	2.20×10^{8}	2.40×10^{8}	6.80×10^{-11}	0.780	7.00×10^{6}
4.2	1.30×10^{-12}	0.900	14.5	0.445	2.80×10^{7}	2.35×10^{8}	2.85×10^{8}	6.00×10^{-11}	0.790	9.00×10^{6}
5.8	1.30×10^{-12}	0.900	16.0	0.440	3.35×10^{7}	2.70×10^{8}	3.20×10^{8}	4.50×10^{-11}	0.790	1.25×10^{7}
7.0	1.30×10^{-12}	0.900	16.0	0.435	3.80×10^{7}	3.10×10^{8}	3.60×10^{8}	4.80×10^{-11}	0.790	1.50×10^{7}
7.8	1.35×10^{-12}	0.900	14.5	0.460	4.05×10^{7}	3.40×10^{8}	4.30×10^{8}	5.50×10^{-11}	0.800	1.60×10^{7}
8.6	1.45×10^{-12}	0.900	16.5	0.460	3.90×10^{7}	3.30×10^{8}	4.15×10^{8}	5.00×10^{-11}	0.800	1.55×10^{7}
9.7	1.50×10^{-12}	0.900	15.0	0.440	4.30×10^{7}	3.80×10^{8}	4.55×10^{8}	4.40×10^{-11}	0.785	2.00×10^{7}
11.1	1.50×10^{-12}	0.900	18.0	0.420	5.30×10^{7}	4.90×10^{8}	5.80×10^{8}	4.00×10^{-11}	0.800	2.30×10^{7}
12.1	1.50×10^{-12}	0.900	18.0	0.420	5.60×10^{7}	5.00×10^{8}	5.90×10^{8}	4.00×10^{-11}	0.800	2.60×10^{7}
13.4	1.50×10^{-12}	0.900	18.0	0.420	5.20×10^{7}	4.80×10^{8}	5.40×10^{8}	4.00×10^{-11}	0.800	2.40×10^{7}
15.0	1.50×10^{-12}	0.900	18.0	0.420	5.20×10^{7}	4.40×10^{8}	5.20×10^{8}	4.00×10^{-11}	0.800	2.20×10^{7}
16.6	1.50×10^{-12}	0.900	16.0	0.420	5.05×10^{7}	4.00×10^{8}	5.25×10^{8}	4.20×10^{-11}	0.830	2.00×10^{7}
18.2	1.55×10^{-12}	0.900	16.0	0.420	4.95×10^{7}	4.00×10^{8}	4.15×10^{8}	4.20×10^{-11}	0.830	1.80×10^{7}
20.0	1.60×10^{-1}	0.900	16.0	0.420	4.70×10^{7}	3.85×10^{8}	4.9×10^{8}	4.20×10^{-11}	0.830	1.50×10^{7}

Table S2. Detailed fitting parameters for the ionic conduction in $LiNH_2$. The CPE_1 and CPE_2 relate to the grain resistance (R_g) and the grain boundary resistance (R_{gb}), respectively.

Pressure (GPa)	CPE1-T	CPE-P	W-T	W-P	R_{gi}	W_R	CPE2-T	CPE2-P	R_{gb}
20.6	1.70×10^{-12}	0.910	6.0	0.375	3.95×10^{7}	1.15×10^{8}	6.80×10^{-11}	0.740	2.75×10^{7}
21.8	1.70×10^{-12}	0.910	6.0	0.375	4.20×10^{7}	1.45×10^{8}	6.80×10^{-11}	0.740	2.85×10^{7}
22.7	1.70×10^{-12}	0.910	9.0	0.375	4.68×10^{7}	1.80×10^{8}	6.80×10^{-11}	0.740	2.95×10^{7}
25.7	1.70×10^{-12}	0.910	13.0	0.375	5.05×10^{7}	1.95×10^{8}	6.80×10^{-11}	0.740	3.05×10^{7}
26.8	1.70×10^{-12}	0.910	13.0	0.375	5.05×10^{7}	1.95×10^{8}	6.80×10^{-11}	0.740	3.05×10^{7}
29.9	1.70×10^{-12}	0.910	13.0	0.375	4.98×10^{7}	1.95×10^{8}	6.80×10^{-11}	0.740	3.10×10^{7}
30.8	1.70×10^{-12}	0.910	13.0	0.375	4.98×10^{7}	1.90×10^{8}	6.80×10^{-11}	0.740	3.00×10^{7}

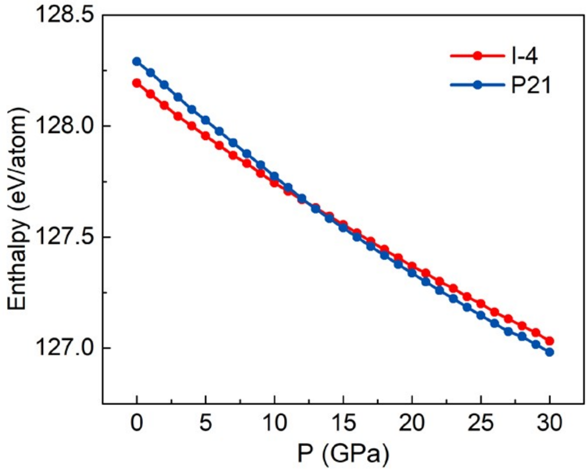

Figure S1. Calculated enthalpies per atom as function of pressure for the tetragonal phase (*I*-4) and the monoclinic phase (*P*21) in $LiNH_2$.

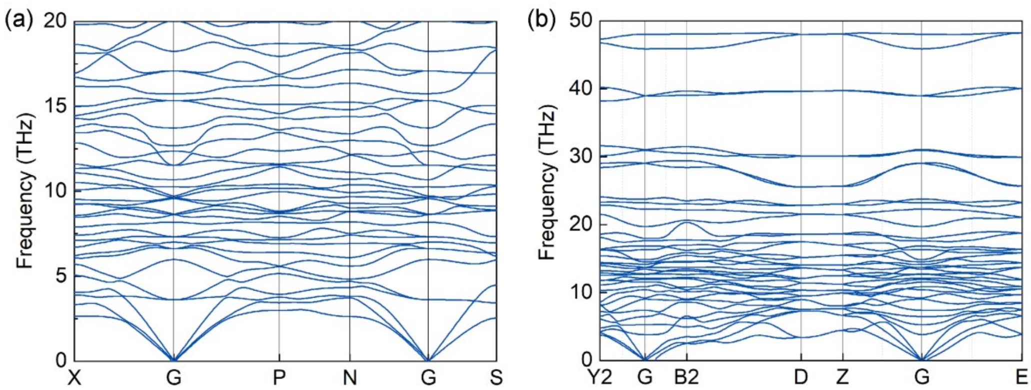

Figure S2. Calculated phonon dispersion of $LiNH_2$ (a) in the tetragonal phase at 0 GPa and (b) in the monoclinic phase at 15 GPa.