Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.
This journal is © the Owner Societies 2022

Supporting Information

Study on superconducting Li-Se-H hydrides

BingYu Li†, WenHua Yang*†, HaiLiang Chen†, Lizhen Zhao†, LingYan Chen†, KaiPing Yang†, WenCai Lu*,†,‡

†College of Physics, Qingdao University, Qingdao, Shandong 266071, P. R. China

‡Institute of Theoretical Chemistry, Jilin University, Changchun, Jilin 130021, P. R. China

*Corresponding author. Email: wencailu@jlu.edu.cn; yangwh@qdu.edu.cn

Table S1 Lattice parameters and atomic fractional coordinates of the $LiSeH_n$ (n=4-10) structures.

Phase	Pressure (GPa)	Parameters (Å, degree)	Atom	Atomic coordinates		
$LiSeH_4$ (*C*2)	150	a=4.38190				
		b=4.43370	H	-0.36380	0.56607	-0.56608
		c=2.75520	H	-0.60630	0.34724	-0.07222
		α=90.0000	Li	0.50000	0.20110	-0.50000
		β=118.6402	Se	-0.50000	0.84927	0.00000
		γ=90.0000				
$LiSeH_4$ (*C*2)	200	a=4.11540				
		b=4.20620	H	-0.36556	0.5609	-0.55481
		c=2.59400	H	-0.61197	0.35051	-0.07383
		α=90.0000	Li	0.50000	0.20333	-0.50000
		β=117.5084	Se	-0.50000	0.85085	0.00000
		γ=90.0000				
$LiSeH_4$ (*C*2)	250	a=4.11540				
		b=4.20620	H	-0.36538	0.55793	-0.55015
		c=2.59400	H	-0.61513	0.35243	-0.07639
		α=90.0000	Li	0.50000	0.20487	-0.50000
		β=117.5084	Se	-0.50000	0.85143	0.00000
		γ=90.0000				
$LiSeH_4$ (*R*-3*m*)	250	a=2.50830				
		b=2.50830	H	0.33333	0.66667	-0.06237
		c=10.81850	H	0.33333	0.66667	0.01118
		α=90.0000	Li	2.00000	1.00000	0.00000
		β=90.0000	Se	0.33333	0.66667	0.16667
		γ=120.0000				
$LiSeH_6$ (*Pmm*2)	200	a=2.85780	H	1.50000	1.15502	0.30232
		b=2.63570	H	0.85232	0.50000	0.24197
		c=3.23420	H	1.00000	0.84705	0.53553
		α=90.0000	Li	0.00000	0.00000	0.02883
		β=90.0000	Se	0.50000	0.50000	0.77305
		γ=90.0000				
$LiSeH_6$ (*Pmm*2)	250	a=2.77130	H	1.50000	1.15739	0.30163
		b=2.57470	H	0.84467	0.50000	0.24100
		c=3.16300	H	1.00000	0.84311	0.53497
		α=90.0000	Li	0.00000	0.00000	0.03351
		β=90.0000	Se	0.50000	0.50000	0.77283
		γ=90.0000				

$LiSeH_6$ (*Pmm*2)	300	a=2.70900	H	1.50000	1.15989	0.30051
		b=2.51840	H	0.83977	0.50000	0.24026
		c=3.10420	H	1.00000	0.83969	0.53493
		α=90.0000	Li	0.00000	0.00000	0.03791
		β=90.0000	Se	0.50000	0.50000	0.77221
		γ=90.0000				
$LiSeH_7$ (*Pm*)	250	a=2.98470	H	-0.49950	-0.13330	0.03784
		b=2.81990	H	-0.04383	0.00000	0.02488
		c=2.96900	H	0.07164	0.00000	-0.19077
		α=90.0000	Li	-0.35179	0.00000	-0.45852
		β=94.2308	H	-1.75111	-0.50000	-0.08612
		γ=90.0000	H	-1.28478	-0.50000	0.02826
			H	-0.29301	-0.50000	-0.23887
			Se	-0.85419	-0.50000	-0.59767
$LiSeH_8$ (*C*2/*m*)	250	a=3.04810	H	0.11349	0.22669	0.20443
		b=4.17360	H	-1.00000	-0.86182	0.00000
		c=5.81460	H	-1.26049	-1.00000	-0.32043
		α=90.0000	Li	-0.50000	0.00000	0.00000
		β=136.0001	Se	-2.00000	-1.00000	-0.50000
		γ=90.0000				
$LiSeH_9$ (*Pmm*2)	300	a=2.98840	H	-0.27450	-0.15255	0.07780
		b=2.57680	H	-0.50000	-1.50000	0.20919
		c=3.37460	H	0.00000	-0.50000	0.30658
		α=90.0000	H	0.00000	0.50000	0.07928
		β=90.0000	H	-0.14347	-1.00000	0.37548
		γ=90.0000	Li	0.00000	-1.00000	0.74472
			Se	-0.50000	-2.50000	0.64684
$LiSeH_{10}$ (*C*2)	250	a=4.96380	H	-0.41148	-0.07922	-0.09224
		b=2.93880	H	-0.61626	-0.63847	-0.76330
		c=5.45150	H	-0.25465	-0.74405	-0.54554
		α=90.0000	H	-0.62548	-0.47137	-0.65962
		β=132.8378	H	-0.12775	-0.69060	-0.35119
		γ=90.0000	Li	0.00000	-0.44730	-0.50000
			Se	-0.50000	0.40656	-1.00000

$LiSeH_{10}$ (*Pm*)	150	a=2.60060 b=4.28140 c=2.93310 α=63.9930 β=90.0188 γ=90.0124	H	-0.03181	0.17239	0.98147
			H	0.13776	0.64826	0.17997
			H	0.46778	0.07917	0.78307
			H	-0.18090	0.29343	0.38755
			H	0.11690	0.29416	0.38487
			H	0.46797	0.13184	0.29681
			H	0.46789	-0.12017	-0.05197
			H	0.79614	-0.35350	1.17664
			H	0.46841	-0.06699	0.33865
			H	-0.03260	-0.02337	0.11201
			Li	-0.03153	0.90845	0.64560
			Se	0.46789	0.50117	0.73374
LiSe (*Cmcm*)	200	a=7.4175 b=2.8296 c=2.7757 α=90.0000 β=89.7564 γ=90.0000	Li	0.07896	0.5	0.24846
			Se	0.35722	-0.5	-0.74755

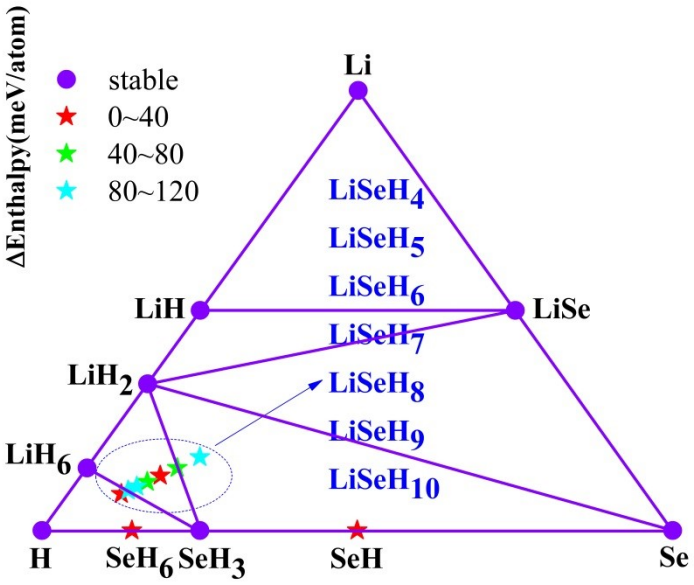

Fig. S1 Triangular phase diagrams of the $LiSeH_n$ (n=4-10) systems at 200 GPa, the corresponding elements and boundary binary phases are chosen from the refs.[1-6] Purple circles and colored stars (red, green and blue stars represent structures with 0~40, 40~80, 80~120 meV/atom above the convex hull) indicated stable and metastable phases, respectively. At 200 GPa, *Pmm*2 $LiSeH_6$ is 22 meV/atom above the convex hull. We performed the structural search for the LiSe at 200 GPa and the results show that the *Cmcm* phase is the most stable structure. The corresponding structural information is given in Table S1.

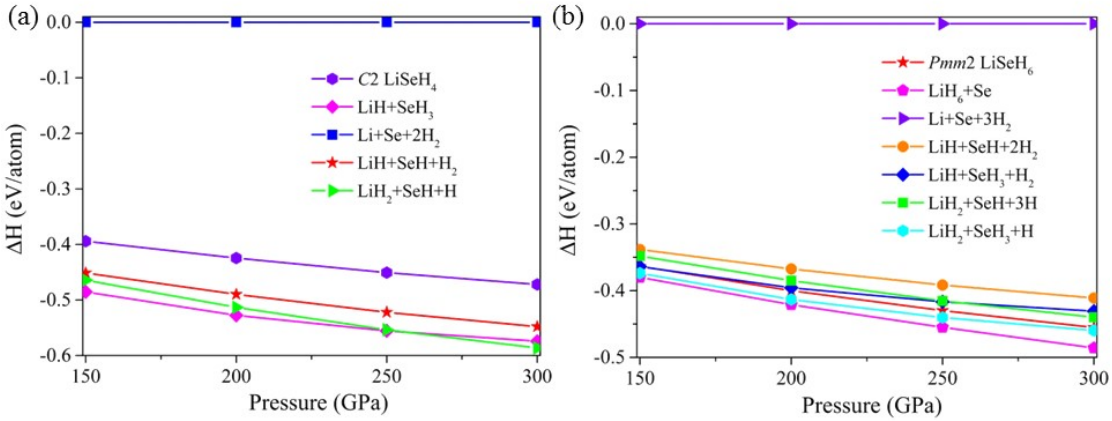

Fig. S2 Enthalpy curves for the $LiSeH_4$ and $LiSeH_6$ as a function of pressure.

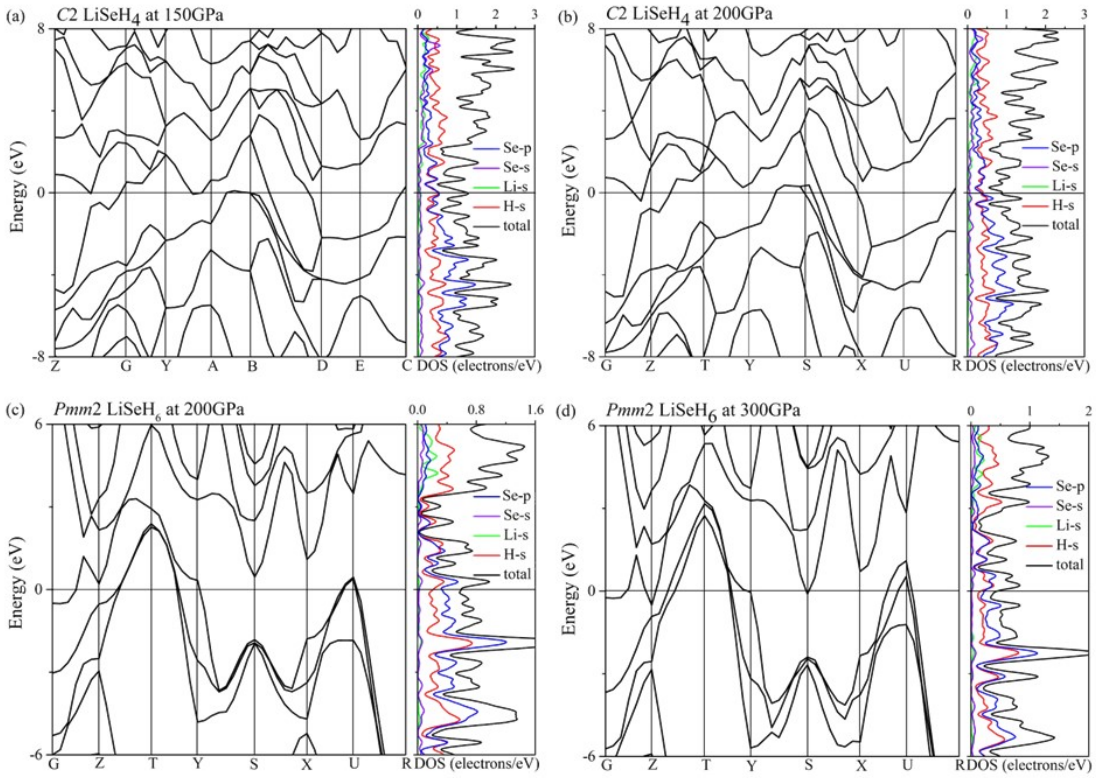

Fig. S3 Calculated electronic band structures and density of states of the predicted crystal structures. (a) *C*2 $LiSeH_4$ at 150 GPa, (b) *C*2 $LiSeH_4$ at 200 GPa, (c) *Pmm*2 $LiSeH_6$ at 200 GPa, and (d) *Pmm*2 $LiSeH_6$ at 300 GPa.

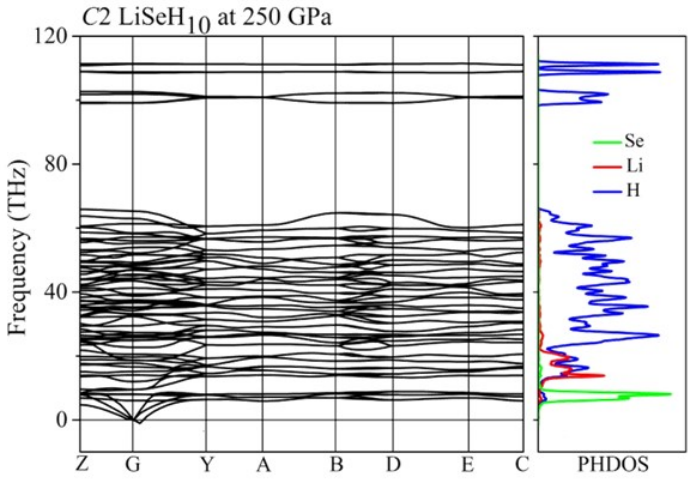

Fig. S4 Phonon dispersion curves, phonon density of states of the predicted crystal structures *C*2 $LiSeH_{10}$ at 250 GPa.

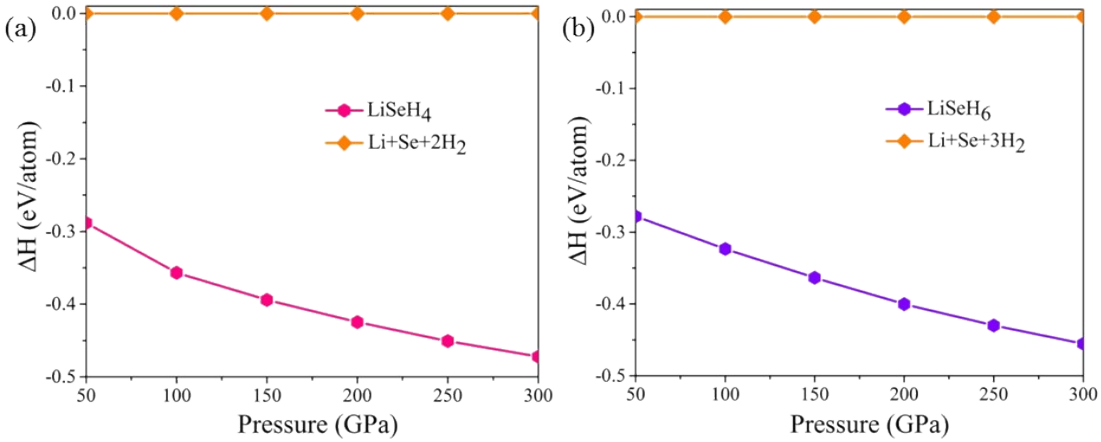

Fig. S5 Enthalpy curves for the $LiSeH_4$ and $LiSeH_6$ as a function of pressure. (a) *C*2 $LiSeH_4$. (b) *Pmm*2 $LiSeH_6$.

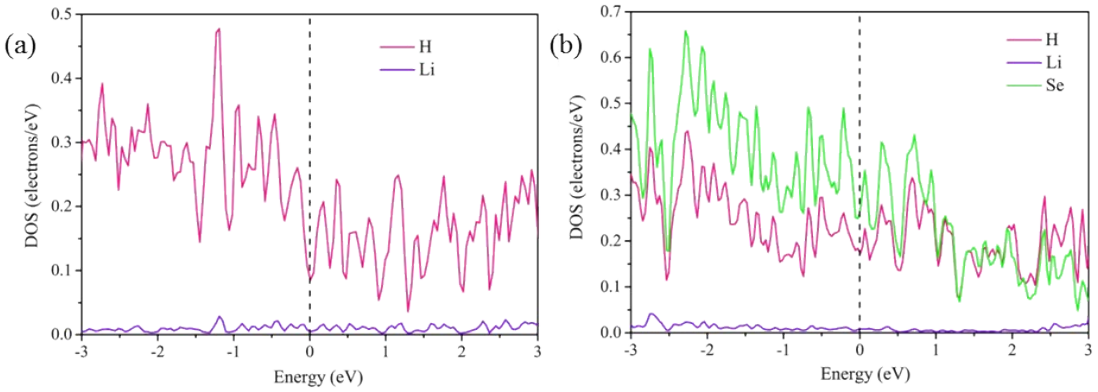

Fig. S6 Density of states of the crystal structures. (a) LiH_6 at 300 GPa, and (b) *Pmm*2 $LiSeH_6$ at 300 GPa.

References

1. S. Zhang, Y. Wang, J. Zhang, H. Liu, X. Zhong, H.-F. Song, G. Yang, L. Zhang and Y. Ma, *Scientific Reports*, 2015, **5**.
2. E. Zurek, R. Hoffmann, N. W. Ashcroft, A. R. Oganov and A. O. Lyakhov, *Proceedings of the National Academy of Sciences of the United States of America*, 2009, **106**, 17640-17643.
3. J. Wu, L.-Z. Zhao, H.-L. Chen, D. Wang, J.-Y. Chen, X. Guo, Q.-J. Zang and W.-C. Lu, *Physica Status Solidi B-Basic Solid State Physics*, 2018, **255**.
4. C. J. Pickard and R. J. Needs, *Nature Physics*, 2007, **3**, 473-476.
5. Y. Ma, A. R. Oganov and Y. Xie, *Physical Review B*, 2008, **78**.
6. Y. Akahama, M. Kobayashi and H. Kawamura, *Physical Review B*, 1993, **47**, 20-26.