

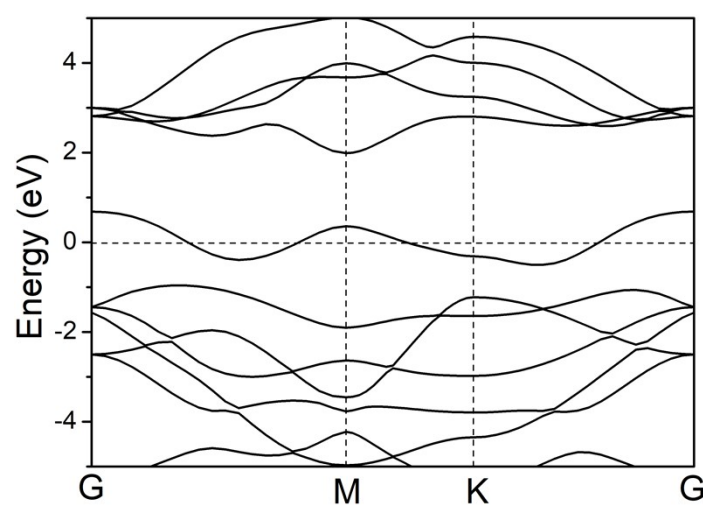
## *Electronic Supplementary Information (ESI) for*

### **Theoretical Study of NbS<sub>2</sub> Monolayer as a Promising Anchoring Material for Lithium-Sulfur Batteries**

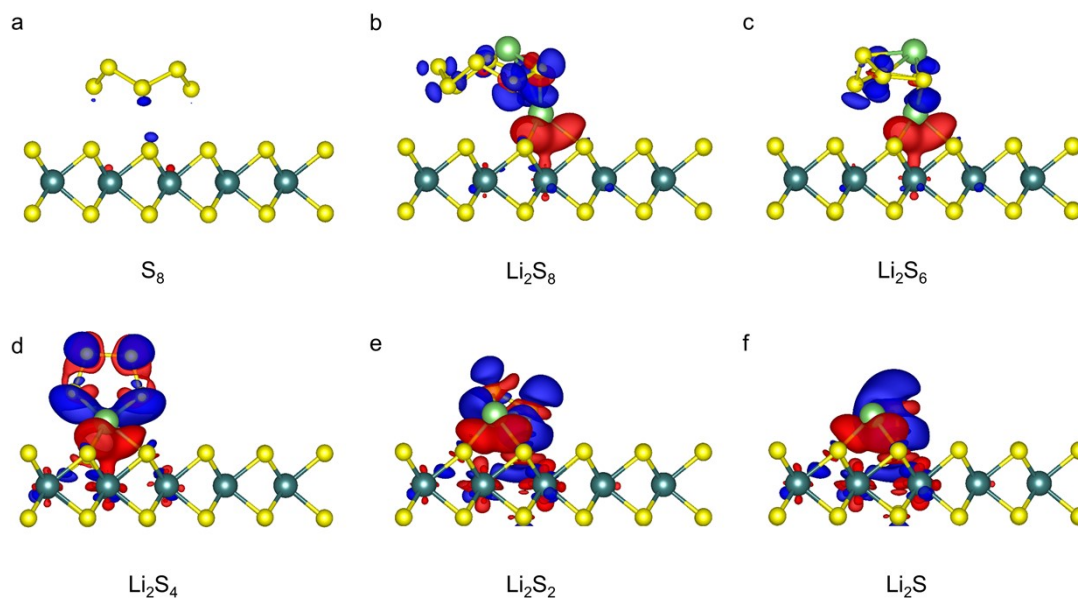
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**Figure S1** Electronic band structures of monolayer NbS<sub>2</sub>.



**Figure S2** (a-f) Charge density difference of LiPSs on NbS<sub>2</sub> monolayer. The electron density is drawn with an isosurface of 0.002 eÅ<sup>-3</sup>. The red surface corresponds to charge accumulation, and the blue one corresponds to charge depletion.

**Table S1** The absorption energy of Li<sub>2</sub>S<sub>4</sub> on NbS<sub>2</sub> with or without dipole moment correction.

	With	Without
Li <sub>2</sub> S <sub>4</sub> -E <sub>ad</sub> (eV)	-2.43	-2.47

**Table S2** The adsorption energies ( $E_{\text{ads}}$ ), the shortest distance between  $\text{S}_8/\text{Li}_2\text{S}_n$  and  $\text{NbS}_2$  ( $d_{\text{a-s}}$ ), the variances of Li-S bond length in LiPSs ( $\Delta d_{\text{Li-S}}$ ), and charge transfer between adsorbates and  $\text{NbS}_2$  ( $Q_{\text{a-s}}$ ).

	$\text{S}_8$	$\text{Li}_2\text{S}_8$	$\text{Li}_2\text{S}_6$	$\text{Li}_2\text{S}_4$	$\text{Li}_2\text{S}_2$	$\text{Li}_2\text{S}$
$E_{\text{ads}}$ (eV)	-0.85	-1.74	-1.61	-2.47	-3.39	-4.38
$d_{\text{a-s}}$ (Å)	3.00	1.62	1.57	1.56	1.66	1.82
$\Delta d_{\text{Li-S}}$ (Å)	0.00	0.11	0.17	0.30	0.28	0.32
$Q_{\text{a-s}}$ (e)	0.09	0.84	0.64	1.00	1.11	1.14

**Table S3** Calculated adsorption energies of  $\text{Li}_2\text{S}_4$  on  $\text{MoS}_2$ ,  $\text{WS}_2$  and  $\text{NbS}_2$ .

	$\text{MoS}_2$	$\text{WS}_2$	$\text{NbS}_2$
$\text{Li}_2\text{S}_4 - E_{\text{ad}}$ (eV)	-0.5	-0.80	-2.47

**Table S4.** Computed zero-point energy (ZPE), entropy corrections (TS), Gibbs free and energy change ( $\Delta G$ ) of critical species on the NbS<sub>2</sub>.

Reaction Step	ZPE (eV)	TS(eV)	Reaction Step	$\Delta G$ (eV)
*S <sub>8</sub>	NA	NA	*S <sub>8</sub> +2Li <sup>+</sup> +2e <sup>-</sup> →*Li <sub>2</sub> S <sub>8</sub>	-3.06
*Li <sub>2</sub> S <sub>8</sub>	0.35	0.33	*Li <sub>2</sub> S <sub>8</sub> →*Li <sub>2</sub> S <sub>6</sub> +1/4S <sub>8</sub>	-0.04
*Li <sub>2</sub> S <sub>6</sub>	0.31	0.39	*Li <sub>2</sub> S <sub>6</sub> →*Li <sub>2</sub> S <sub>4</sub> +1/4S <sub>8</sub>	-0.60
*Li <sub>2</sub> S <sub>4</sub>	0.25	0.42	*Li <sub>2</sub> S <sub>4</sub> →*Li <sub>2</sub> S <sub>2</sub> +1/4S <sub>8</sub>	0.18
*Li <sub>2</sub> S <sub>2</sub>	0.17	0.37	*Li <sub>2</sub> S <sub>2</sub> →*Li <sub>2</sub> S+1/8S <sub>8</sub>	0.09
*Li <sub>2</sub> S	0.14	0.19		

### Coordinates for Structures

S<sub>8</sub>

```

16.6709995270      0.0000000000      0.0000000000
-8.3354997635     14.4375090968      0.0000000000
0.0000000000      0.0000000000     20.0000000000

```

Nb S

25 58

Direct

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0.333163004      0.264559013      0.222896004

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0.0000000000	0.0000000000	20.0000000000

Li S Nb

2 58 25

Direct

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Li<sub>2</sub>S<sub>6</sub>

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0.0000000000	0.0000000000	20.0000000000

Li S Nb

2 56 25

Direct

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Li<sub>2</sub>S<sub>4</sub>

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0.0000000000	0.0000000000	20.0000000000

Li S Nb

2 54 25

Direct

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0.400234997	0.599947993	0.304729009
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0.599008978	0.799037017	0.305279994
0.799935993	0.800376024	0.149253988
0.799783989	0.799650010	0.304661012
0.492117024	0.381536004	0.447699022
0.369845993	0.153499011	0.455824995
0.391976005	0.199682003	0.547412968
0.470932034	0.346847018	0.541858006
0.133435996	0.066134997	0.225853992
0.331064998	0.062265002	0.222593999
0.532899073	0.066552001	0.225482988
0.731805968	0.064531001	0.227002001
0.932951964	0.065945002	0.227055001
0.135207003	0.269755999	0.226391006

0.331824017	0.268593029	0.221502018
0.537063002	0.268828995	0.221701002
0.732541986	0.269165018	0.226364994
0.934922995	0.268379009	0.227025008
0.135443024	0.467394018	0.226966000
0.331218015	0.466892031	0.225659990
0.534828027	0.468690024	0.224765015
0.734011966	0.466401009	0.225979996
0.932799005	0.468395021	0.227032995
0.133096985	0.667125992	0.226620007
0.331497036	0.664224049	0.226447010
0.534002013	0.665911961	0.226283002
0.730847995	0.665181984	0.226640987
0.933783023	0.665089044	0.226745987
0.136732007	0.869295043	0.226015997
0.332071003	0.869268027	0.225843000
0.536296993	0.869213993	0.226606989
0.733029049	0.868703055	0.227120996
0.934301963	0.869683052	0.226849008

Li<sub>2</sub>S<sub>2</sub>

16.6709995270	0.0000000000	0.0000000000
-8.3354997635	14.4375090968	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Li S Nb

2 52 25

Direct

0.426695008	0.305510027	0.396427989
0.681463003	0.304062028	0.395694995
0.000890000	0.000913000	0.148378003



0.000336000	0.000009000	0.305258012
0.200061001	0.000564000	0.149326992
0.200359993	0.000081000	0.304486990
0.399363055	0.999125062	0.146780992
0.399576029	0.998923064	0.306497002
0.600393003	0.000520000	0.148912001
0.600045020	0.000366000	0.304129982
0.800059036	0.000913000	0.148176003
0.798897989	0.000135000	0.305084991
0.000656001	0.201187007	0.149189997
0.000282003	0.201317004	0.305218005
0.200437993	0.200449004	0.147216010
0.201734006	0.200829004	0.306739998
0.398553985	0.199500994	0.147753000
0.398617998	0.198897018	0.305531001
0.600561016	0.199552997	0.147503996
0.599915981	0.198643002	0.305206013
0.799983966	0.200772014	0.146887004
0.798905024	0.200956012	0.306531000
0.000511011	0.400510032	0.150205994
0.000137009	0.400543027	0.304888988
0.200188008	0.400489026	0.150312006
0.200328997	0.400290992	0.305011988
0.397803025	0.399681005	0.147593999
0.401129983	0.400451012	0.306502008
0.600445999	0.400661001	0.153303003
0.601507990	0.403019011	0.296373987
0.802022010	0.399741016	0.147443998
0.799566017	0.400437008	0.306407976
0.001757005	0.600359980	0.147262001

0.001524997	0.601490055	0.306537008
0.200772012	0.600990016	0.148020995
0.201093016	0.601795032	0.306643009
0.398811980	0.600453977	0.147477996
0.400209002	0.601466010	0.306745005
0.601281005	0.603115016	0.145706999
0.601490972	0.602129008	0.304818010
0.801923978	0.603122017	0.145560992
0.800961948	0.602256032	0.304778004
0.000748024	0.800934060	0.149285007
0.000256996	0.800357991	0.303472018
0.200769038	0.799230031	0.147838998
0.201033002	0.799601988	0.305675006
0.398829005	0.799174016	0.147835994
0.399213997	0.799823009	0.305799007
0.600186999	0.800866023	0.149215996
0.600243992	0.800470021	0.303437996
0.800295003	0.800567981	0.146106005
0.799189016	0.798813023	0.305467987
0.609417014	0.421838007	0.404215002
0.550665951	0.297422015	0.451449013
0.134057004	0.069175000	0.227051997
0.335938973	0.066248002	0.226693010
0.530249011	0.066187004	0.226310992
0.735077026	0.069459004	0.226557994
0.933133991	0.066573002	0.227017999
0.134440005	0.265298998	0.227307010
0.332971020	0.267056004	0.225784993
0.529851984	0.259929014	0.225832009
0.733849017	0.267077009	0.225537992

0.930705002	0.265442999	0.227121997
0.135141996	0.470143010	0.227719998
0.336507011	0.469807019	0.227653003
0.530166973	0.472952012	0.224283004
0.743052001	0.473003007	0.224235010
0.933531021	0.469854018	0.227460003
0.132790987	0.665952981	0.227007008
0.333519035	0.666073070	0.227186990
0.530726060	0.663781016	0.226181006
0.733777016	0.667367028	0.224943995
0.933265972	0.663750036	0.226047993
0.135765006	0.866023059	0.226631999
0.334376025	0.868418027	0.226657009
0.530550038	0.866211052	0.226510000
0.735921069	0.867135034	0.226177001
0.931095050	0.867016993	0.226301003

Li<sub>2</sub>S

16.6709995270	0.0000000000	0.0000000000
-8.3354997635	14.4375090968	0.0000000000
0.0000000000	0.0000000000	20.0000000000

Li S Nb

2 51 25

Direct

0.432537981	0.314678010	0.389039993
0.683449949	0.314334027	0.388673019
0.000228026	0.999727024	0.149057007
0.000358043	0.999720022	0.305777025
0.199130024	0.999388028	0.149313998
0.200630058	0.999609049	0.304612994

0.398957054	0.998074055	0.146316004
0.399350004	0.998454996	0.306200004
0.600258022	0.999460028	0.148844004
0.599398033	0.999847046	0.304224014
0.799664954	0.999812037	0.148707008
0.798618045	0.999787002	0.305464005
0.000274001	0.200159005	0.149313998
0.000036003	0.200922010	0.305353999
0.200042993	0.199760014	0.147479999
0.201590007	0.200373007	0.306912994
0.396780009	0.198111009	0.146952009
0.399930009	0.198525011	0.305023003
0.600944965	0.197971005	0.146597993
0.598874970	0.198407003	0.304800010
0.799832017	0.199906013	0.146867013
0.798650003	0.200609006	0.306422997
0.000425004	0.399620003	0.149734998
0.000006005	0.399998995	0.304579997
0.199660000	0.399657027	0.150142002
0.199745016	0.399940041	0.304944015
0.397588021	0.399260034	0.148092997
0.399462015	0.400362035	0.306501007
0.600174017	0.400879017	0.154363012
0.600212006	0.399777016	0.297400999
0.801875983	0.399281007	0.147367001
0.801179023	0.400473008	0.305685997
0.001519015	0.600498961	0.146994996
0.001321006	0.600525977	0.306604004
0.200648008	0.600578029	0.147760999
0.200493003	0.600905003	0.306643987

0.399069019	0.600303040	0.147566009
0.399377023	0.600810015	0.307114983
0.601035040	0.602298043	0.146859002
0.600499981	0.600630014	0.306180000
0.801380996	0.602456972	0.146482003
0.800297988	0.600285007	0.305693007
0.000092983	0.800149983	0.149979997
0.000120002	0.799277062	0.304215002
0.200222026	0.798638043	0.147880006
0.200905986	0.798672986	0.305676007
0.398647003	0.798466035	0.147927999
0.398701029	0.799100034	0.305864000
0.599942053	0.799788000	0.149897993
0.599708014	0.799860000	0.304110003
0.799796006	0.799317026	0.147394001
0.798825989	0.798111054	0.306405020
0.598517006	0.395470011	0.399445009
0.133901005	0.068447004	0.227318001
0.335350027	0.065026003	0.226146007
0.529767997	0.065009997	0.225913000
0.734544009	0.068705999	0.226706004
0.932826017	0.065882001	0.227470994
0.134235009	0.264864007	0.227450991
0.332645002	0.266326026	0.226020002
0.529174964	0.258212005	0.223225999
0.733606019	0.266366997	0.225379014
0.930523971	0.264941011	0.227003002
0.134951009	0.469803023	0.227379990
0.335820991	0.469787004	0.227455997
0.529619967	0.472197000	0.225378013

0.742645049	0.472090023	0.224698019
0.934219013	0.469819999	0.226710010
0.132591993	0.665216993	0.226876998
0.332973027	0.665382065	0.227243996
0.530132996	0.662835038	0.227068996
0.733071006	0.665992020	0.226559997
0.932901987	0.662783977	0.226639009
0.135451014	0.865252061	0.227010989
0.334064035	0.867682038	0.226531005
0.530162981	0.865509016	0.226775002
0.735447020	0.866297056	0.227020001
0.930795033	0.866159992	0.227347994