

Prediction of Be₂B₂ monolayer: An ultrahigh capacity anode material for Li-ion and Na-ion batteries

Yao Wu^a and Jianhua Hou^{*a,b}

^aSchool of Materials Science and Engineering, Changchun University of Science and Technology, Changchun, 130022, PR China.

^bEngineering Research Center of Optoelectronic Functional Materials, Ministry of Education, Changchun 130022, PR China.

Corresponding author: houjh163@163.com

Supporting Information:

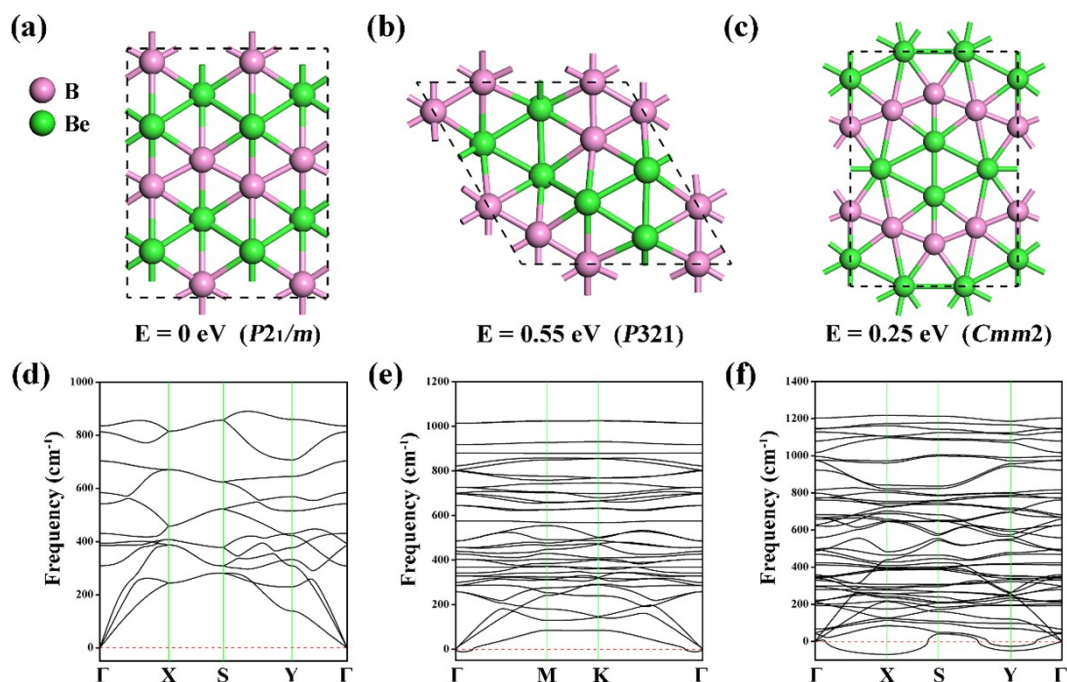


Fig. S1. Optimized low-energy Be_2B_2 structures with space group (a) $P2_1/m$, (b) $P321$ and (c) $Cmm2$. Unit cell is plotted with dotted black lines, and the calculated relative energies are labeled down below. The corresponding phonon dispersion curves for the above structures with space group (d) $P2_1/m$, (e) $P321$ and (f) $Cmm2$.

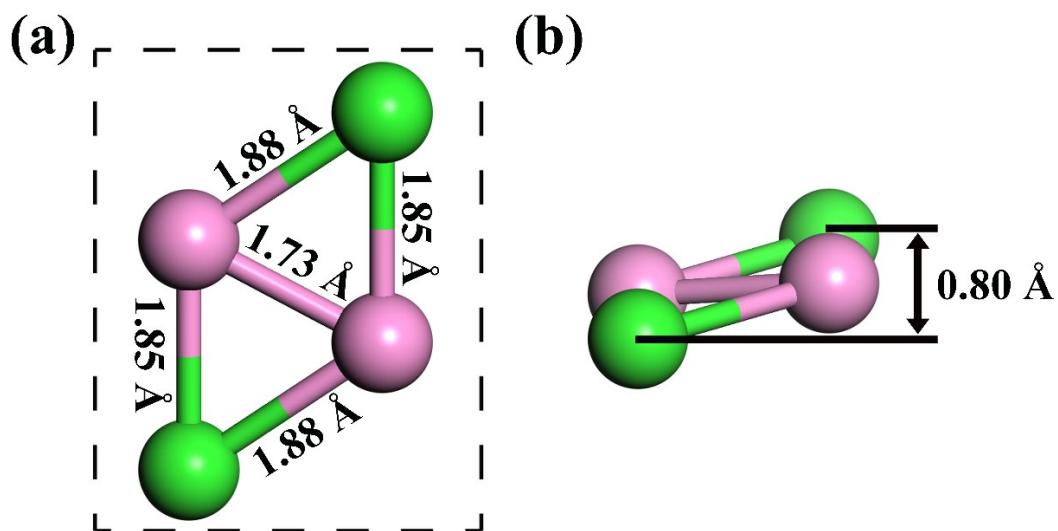


Fig. S2. (a) Bond lengths and (b) thickness are marked in the optimized unit structure of Be_2B_2 monolayer.

Table S1. Summary of the initial site, final site, adsorption energy and adsorption height for Li/Na atom adsorbed on the Be₂B₂ monolayer surface.

Metal adatoms	Initial sites	Final sites	Adsorption energies (eV)	Adsorption heights (Å)
Li	T1	B1	-2.16	2.364
	T2	T2	-2.01	2.339
	T3	B1	-2.16	2.360
	T4	B1	-2.16	2.361
	B1	B1	-2.16	2.357
Na	T1	B1	-1.29	2.778
	T2	T2	-1.24	2.658
	T3	B1	-1.29	2.773
	T4	T4	-1.10	2.515
	B1	B1	-1.29	2.778

In addition, we provide the detailed coordinate information of Be₂B₂ and Li_x/Na_xBe₂B₂ ($x = 0.5, 1.0, 1.5$ and 2.0), as follows:

Lattice parameter (both Be₂B₂ and Li_x/Na_xBe₂B₂):

6.1000000000000000	0.0000000000000000	0.0000000000000000
0.0000000000000000	7.5800000000000000	0.0000000000000000
0.0000000000000000	0.0000000000000000	20.0000000000000000

Coordinate information (Be₂B₂):

Be	0.1234896759016390	0.1859650687335090	0.5069894692500011
Be	0.3734810555737700	0.3145754596306071	0.4671893318000001
Be	0.6234896759016390	0.1859650687335090	0.5069894692500001
Be	0.8734810555737710	0.3145754596306071	0.4671893318000011
Be	0.1234896759016390	0.6859650687335103	0.5069894692500011
Be	0.3734810555737700	0.8145754596306082	0.4671893318000001
Be	0.6234896759016390	0.6859650687335103	0.5069894692500001
Be	0.8734810555737710	0.8145754596306082	0.4671893318000011
B	0.1234832362295080	0.4470852799472301	0.4893645220500001
B	0.3733430744262300	0.0534550143799473	0.4848143234000011
B	0.6234832362295080	0.4470852799472301	0.4893645220500001

B	0.8733430744262301	0.0534550143799473	0.4848143234000011
B	0.1234832362295080	0.9470852799472312	0.4893645220500011
B	0.3733430744262300	0.5534550143799482	0.4848143234000001
B	0.6234832362295080	0.9470852799472312	0.4893645220500011
B	0.8733430744262301	0.5534550143799482	0.4848143234000001

Coordinate information (Li_{0.5}Be₂B₂):

Li	0.3712377495081970	0.4167184666226921	0.5798209732000001
Li	1.6256059383606600	0.0833678093667547	0.3949895515000000
Be	0.1256165801639340	0.1869757608179421	0.5069851151500001
Be	0.3760717463934430	0.3131282730870710	0.4633357712500000
Be	0.6199815236065570	0.1874155754617420	0.5118466037000001
Be	0.8705471080327870	0.3136295218997360	0.4683240576000001
Be	0.1265313567213110	0.6863408835092362	0.5051027482500011
Be	0.3769481259016390	0.8145063625329821	0.4648111326500001
Be	0.6190205978688530	0.6860573625329821	0.5103857078000001
Be	0.8696736522950821	0.8141902749340381	0.4703500618500011
B	0.1243085881967210	0.4451587841688661	0.4907310128000001
B	0.3743025821311480	0.0546970799472296	0.4821278079000010
B	0.6217520800000000	0.4458901005277051	0.4931598372000001
B	0.8717867878688530	0.0554306449868075	0.4845501025000011
B	0.1238459331147540	0.9463583319261232	0.4882007099500011
B	0.3740117657377051	0.5565646840369402	0.4805739589500001
B	0.6219264609836070	0.9439644795514522	0.4946664314500011
B	0.8722414229508200	0.5542233626649081	0.4871384163500001

Coordinate information (Li_{1.0}Be₂B₂):

Li	0.3691737200000000	0.4080551906332461	0.5805052721000001
Li	0.8763749918032791	0.4082559071240111	0.5804945777500001
Li	0.6228857593442621	0.0824251639841689	0.3945913630500000
Li	1.6229294891803303	0.5671542389182062	0.3961268701500001
Be	0.1226682996721310	0.1925761258575200	0.5089821390500011
Be	0.3802970165573770	0.3161868186015830	0.4584103960000001
Be	0.6226954801639349	0.1910097899736151	0.5152768833000001
Be	0.8650589983606561	0.3161705548812671	0.4583851501000001
Be	0.1225935068852460	0.6879500957783651	0.5081002506000001
Be	0.3794034360655740	0.8151550726912942	0.4660834466000001
Be	0.6226838160655740	0.6883974565963061	0.5179603544000001
Be	0.8658863850819671	0.8151531154353572	0.4660230366500011
B	0.1225695391803280	0.4457010715039581	0.4918382161500011
B	0.3742910085245900	0.0573491010554090	0.4841655117500011

B	0.6226034506557380	0.4468935970976261	0.5003914671500002
B	0.8708949614754101	0.0573578486807389	0.4840852017500011
B	0.1226006552459020	0.9499905625329832	0.4885969318000011
B	0.3743632032786890	0.5577750784960432	0.4818960605500001
B	0.6225952937704921	0.9475240926121391	0.4970191167500011
B	0.8707728275409841	0.5577912604221641	0.4818677544000001

Coordinate information (Li_{1.5}Be₂B₂):

Li	0.3693982031147541	0.4216806178100271	0.5833312950500001
Li	0.8745162857377050	0.4217890353562011	0.5833175433500001
Li	0.6219123008196720	0.5803977674142481	0.3967102833000001
Li	0.3694294514754101	0.9221240486807392	0.5833179166500001
Li	0.6218972718032790	0.0804860039577837	0.3966706605000001
Li	0.8745137495081971	0.9230542414248032	0.5833792810000001
Be	0.1218731044262300	0.1877277093667551	0.5162592853000011
Be	0.3736465201639341	0.3117559804749341	0.4608741735000000
Be	0.6220637509836070	0.1867343924802111	0.5186701903500011
Be	0.8702654890163940	0.3117783773087071	0.4608041270000001
Be	0.1219314567213110	0.6877413678100272	0.5162764955500011
Be	0.3736826344262301	0.8117350873350931	0.4608943347500001
Be	0.6219956572131150	0.6867513451187343	0.5186771061000001
Be	0.8702301098360661	0.8117311415567291	0.4608923341500011
B	0.1219456145901640	0.4450828141160961	0.4921931172000001
B	0.3722100049180330	0.0555385989445911	0.4802529277500011
B	0.6219599931147540	0.4432044221635891	0.4972801323000002
B	0.8716957172131151	0.0555477854881267	0.4801957347000011
B	0.1219571547540980	0.9450980960422182	0.4921585262000011
B	0.3722094985245900	0.5555331937994731	0.4803059616500001
B	0.6219564011475410	0.9432514436675472	0.4972621421500011
B	0.8716856259016390	0.5555183634564651	0.4802864315500001

Coordinate information (Li_{2.0}Be₂B₂):

Li	0.3719228196721310	0.4224683539577840	0.5829248126500001
Li	0.8719388968852460	0.4224382864116101	0.5829254085500001
Li	0.6219467455737711	0.5772376906332462	0.3941113454000001
Li	1.1219837618032800	0.5770868221635891	0.3940616132500001
Li	0.3722676570491801	0.9226568874670192	0.5829445996500001
Li	0.6218643814754100	0.0769598035620053	0.3940913349500000
Li	0.8716425624590170	0.9226562576517162	0.5829452574000001
Li	0.1219601321311480	0.0768907170184697	0.3940903437500001
Be	0.1219291252459020	0.1878595787598951	0.5191126027000012

Be	0.3719010681967210	0.3118340945910291	0.4583588132500001
Be	0.6218900650819671	0.1878635153034301	0.5191147172500001
Be	0.8718803963934430	0.3118331336411611	0.4583592429500001
Be	0.1218680965573770	0.6877712538258581	0.5192068915000011
Be	0.3717904857377050	0.8116851188654363	0.4584236248000001
Be	0.6218189636065580	0.6877572014511882	0.5191794768000001
Be	0.8718593562295081	0.8116649873350941	0.4584434100500011
B	0.1218556824590160	0.4436774081794201	0.4972283415000001
B	0.3718374259016390	0.0558675320580476	0.4802193313000011
B	0.6218399429508200	0.4436771445910291	0.4972278826000001
B	0.8718401406557380	0.0558753799472297	0.4802199648500011
B	0.1218633421311480	0.9437084084432732	0.4972459628000011
B	0.3718661713114750	0.5559349952506602	0.4802476412000001
B	0.6218489363934430	0.9436814250659642	0.4972290320500011
B	0.8718638439344260	0.5559340039577841	0.4802483487500001

Coordinate information (Na_{0.5}Be₂B₂):

Be	0.1235080429508200	0.1862843456464380	0.5072470749500011
Be	0.3736536963934430	0.3135107860158310	0.4659472474000001
Be	0.6223453921311480	0.1868050530343010	0.5094834350500002
Be	0.8726945132786890	0.3140591866754621	0.4682316146500001
Be	0.1243925055737710	0.6862182882585761	0.5061015761000001
Be	0.3740839206557380	0.8142197246701852	0.4672087492000001
Be	0.6217461695081971	0.6860415488126651	0.5080347607000001
Be	0.8718115849180331	0.8139808997361492	0.4694147425500000
B	0.1231467050819670	0.4458981346965701	0.4906629118500001
B	0.3730686398360660	0.0545778730870713	0.4837139645500000
B	0.6229558734426230	0.4456649562005281	0.4917070426500000
B	0.8729556768852460	0.0544437862796835	0.4847226041000011
B	0.1232868460655740	0.9459475686015852	0.4898507286500011
B	0.3732020521311480	0.5560279470976262	0.4821312622500001
B	0.6227934086885250	0.9442786402374682	0.4930045283000011
B	0.8727485834426230	0.5543343539577841	0.4856321178000001
Na	0.3711558968852460	0.4202224675461741	0.6045870709500001
Na	1.6258604921311499	0.0821021977572560	0.3694185683000001

Coordinate information (Na_{1.0}Be₂B₂):

Be	0.1224826067213110	0.1906265043535620	0.5081300153500001
Be	0.3758726429508200	0.3161783856200531	0.4614775900500001
Be	0.6224207080327872	0.1906355538258580	0.5121443403500001
Be	0.8689849018032790	0.3161123887862801	0.4614763232500000

Be	0.1224040763934430	0.6881864877308711	0.5084720532500001
Be	0.3758363534426230	0.8157858986807393	0.4669151435500001
Be	0.6225262352459020	0.6881612295514521	0.5141931385500002
Be	0.8691085498360661	0.8157956522427452	0.4668372907000011
B	0.1224041742622950	0.4473968928759901	0.4909943012500000
B	0.3729231459016390	0.0565131439313985	0.4849291805000011
B	0.6223939242622950	0.4472633460422171	0.4956171022500001
B	0.8719581803278691	0.0565680749340370	0.4848296274500011
B	0.1224128177049180	0.9493799212401072	0.4903583120500011
B	0.3730690518032790	0.5573591583113461	0.4827716782000001
B	0.6224985147540980	0.9480240788918223	0.4949903953000012
B	0.8717890770491801	0.5573442492084442	0.4827484688500001
Na	0.3720466278688521	0.4120702025065971	0.6108067008000001
Na	0.8726806760655741	0.4122888423482851	0.6107318194000001
Na	0.6227764501639340	0.0769277125329816	0.3659071392000001
Na	1.6223885919672103	0.5710439428759901	0.3664693797500001

Coordinate information (Na_{1.5}Be₂B₂):

Be	0.1217735796721310	0.1869693647757261	0.5104019859500011
Be	0.3732674129508201	0.3118684563324541	0.4607018476500001
Be	0.6217815418032792	0.1864136783641160	0.5134655740000002
Be	0.8702794870491801	0.3119756833773091	0.4607965583500011
Be	0.1217574767213110	0.6870149315303442	0.5103852349500001
Be	0.3732353624590160	0.8118838744063333	0.4608151876000001
Be	0.6218545078688530	0.6864250998680742	0.5134862960000001
Be	0.8702568649180331	0.8120051035620062	0.4607518581000011
B	0.1217638703278690	0.4456421994722961	0.4882604364000001
B	0.3720632962295080	0.0539638126649077	0.4791538326500011
B	0.6217435486885250	0.4442869452506601	0.4919538404000001
B	0.8714640370491800	0.0540028105540898	0.4792252278000011
B	0.1217507526229510	0.9456172519788932	0.4882704646000011
B	0.3720868490163940	0.5539654208443281	0.4792121924000001
B	0.6217132706557380	0.9442946600263872	0.4919343651000011
B	0.8714528450819671	0.5540330205804761	0.4792060330500001
Na	0.3710857773770490	0.4270983279683381	0.6108355520500001
Na	0.8725302919672131	0.4271332294195251	0.6108560783500001
Na	0.6218712306557380	0.5736324023746711	0.3643156827500000
Na	0.3710311616393440	0.9271306751978903	0.6108503062000001
Na	0.6218099981967210	0.0741597076517151	0.3642785098000001
Na	0.8725159114754100	0.9279370113456472	0.6108529358000001

Coordinate information (Na_{2.0}Be₂B₂):

Be	0.1218902175409840	0.1874613373350930	0.5156772744500011
Be	0.3718845891803280	0.3121857245382591	0.4616351876500001
Be	0.6218809480327872	0.1874721591029021	0.5156656741000001
Be	0.8718879844262300	0.3121927965699211	0.4616387516500001
Be	0.1218951357377050	0.6874220182058061	0.5157070103000011
Be	0.3718824814754100	0.8121239109498692	0.4616573060000001
Be	0.6218784990163930	0.6874357271767821	0.5157121014500001
Be	0.8718908637704920	0.8121236361477581	0.4616663110500011
B	0.1218880434426230	0.4451346903693941	0.4948689891500001
B	0.3718852803278691	0.0544435571240106	0.4824887334000000
B	0.6218853114754100	0.4451421952506601	0.4948681469000001
B	0.8718862393442620	0.0544463199208444	0.4824905021000011
B	0.1218873818032790	0.9451471416886561	0.4948604080000011
B	0.3718872100000000	0.5544545056728241	0.4825057931000001
B	0.6218851973770490	0.9451478170184712	0.4948603258500011
B	0.8718862663934430	0.5544581192612141	0.4825087578000001
Na	0.3718865832786890	0.4268977241424811	0.6135342870500001
Na	0.8718878906557381	0.4268977056728231	0.6135342702000001
Na	0.6218886481967210	0.5726859456464382	0.3638077666500000
Na	1.1218864900000001	0.5726298378627971	0.3638077470500001
Na	0.3719105991803280	0.9269601787598952	0.6135276875000001
Na	0.6218871845901640	0.0726126940633246	0.3638027315500000
Na	0.8718629237704921	0.9269677040897101	0.6135285090000001
Na	0.1218880304918030	0.0725765532981531	0.3638057281000001