

Supporting Information of

**Dirac nodal surface semimetallic carbon based structure as
a universal anode material for metal-ion batteries with high
performance**

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Figure S1. (a) The total potential energies at the temperature of 300 and 2000 K during 10 ps. (b) The snapshot of 300 K for bct-C56 at the end of 10 ps. (c) The snapshot of 2000 K for bct-C56 at the end of 10 ps.

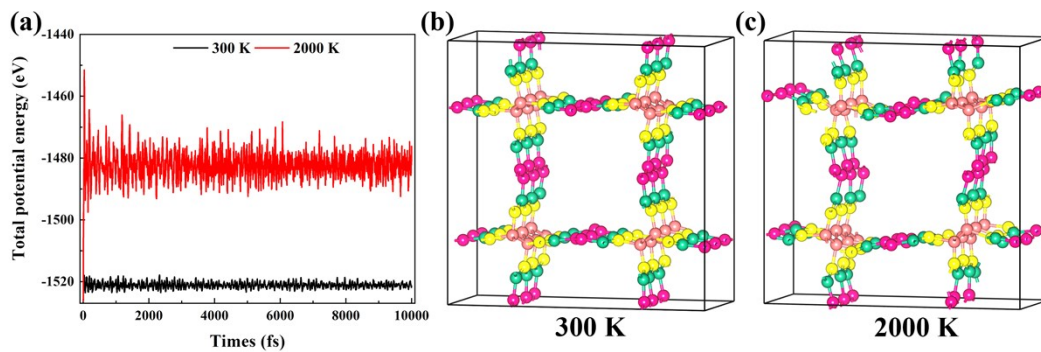


Figure S2. The band structures of bct-C56 at the high symmetry points along the line X-Z₁, X-N, M-P, and Γ -N.

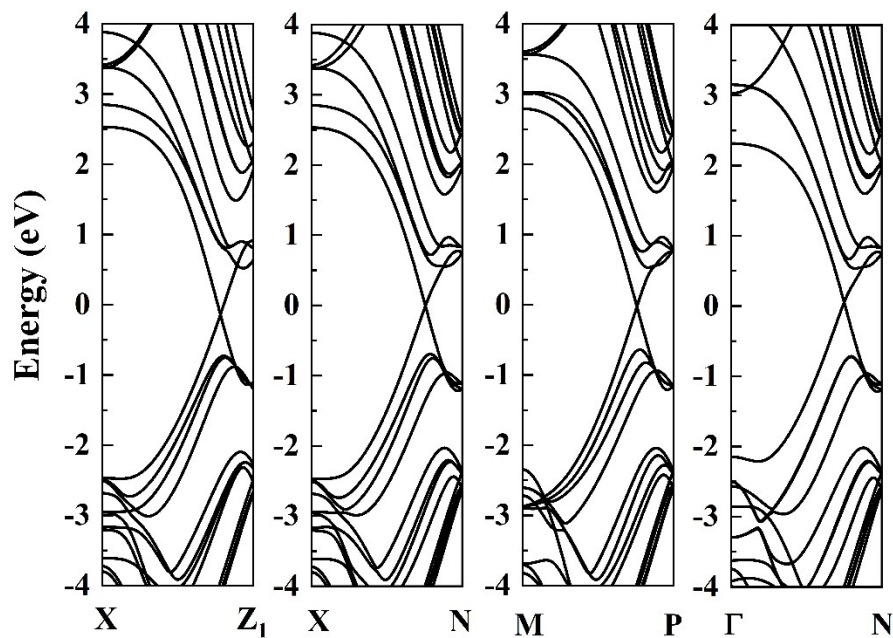


Figure S3. The 3D band structure of bct-C56 along the X-P-N-N₁ plane.

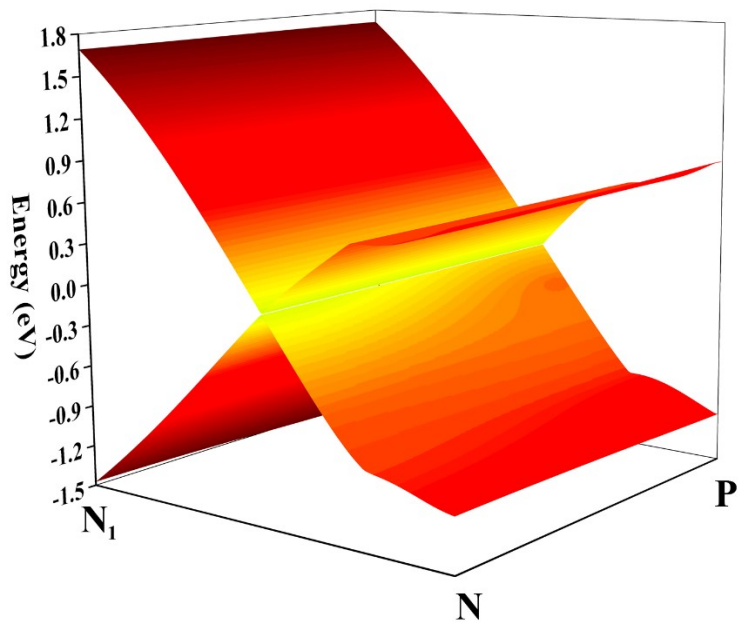


Figure S4. The band structure of bct-C56 by considering SOC effect.

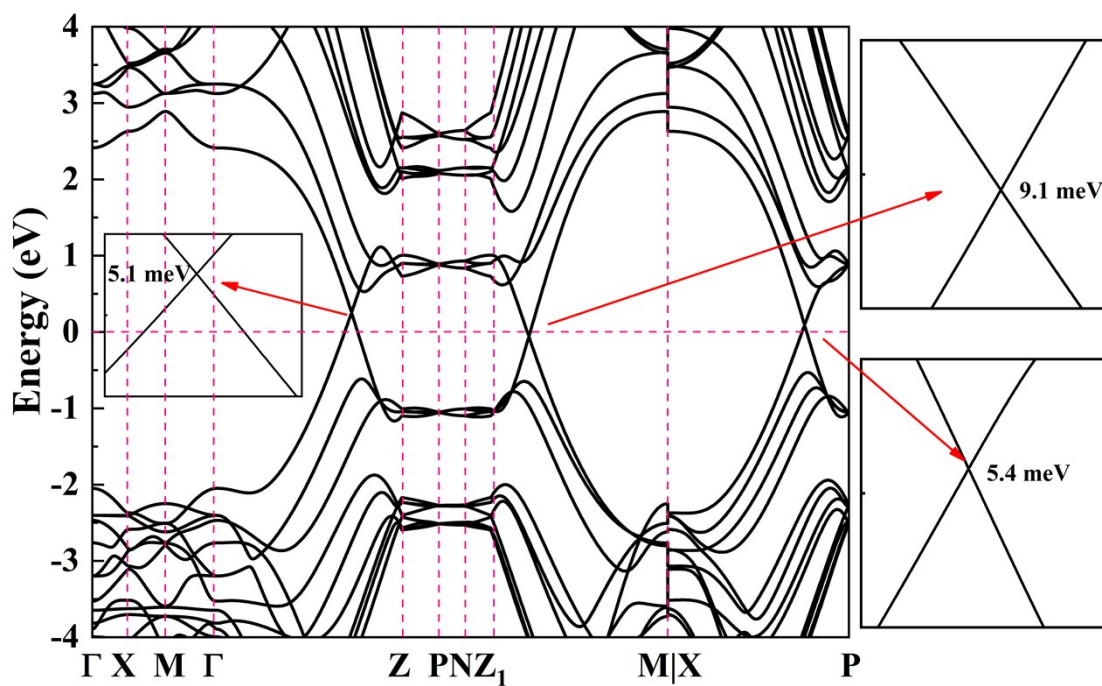
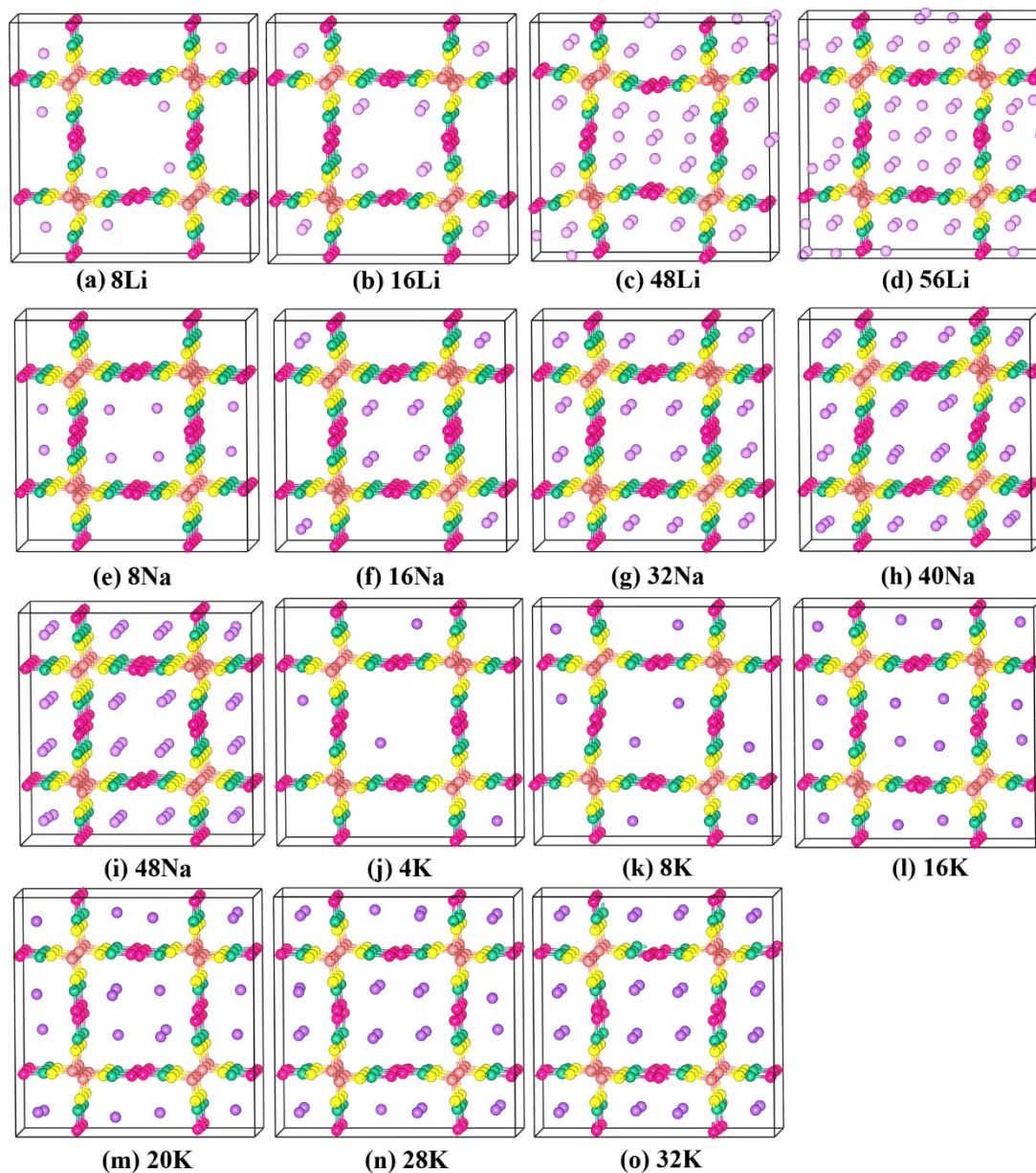


Figure S5. The most stable structures at different concentration (a-d) Li-, (e-i) Na-, and (j-o) K-ions in 3D porous bct-C56.



The cif file of bct-c56 in vasp format.

Bct-c56

1.0000000000000000

17.2424489297253452 0.0000000000000000 0.0000000000000000

-0.0000000000000000 17.2424489297253452 -0.0000000000000000

0.0000000000000000 0.0000000000000000 2.4672389730169195

C

56

Direct

0.2564389031128460 0.9795244009786973 0.0000000000000000

0.7435610668871516 0.0204755990213025 -0.0000000000000000

0.0204755990213025 0.2564389031128460 -0.0000000000000000

0.9795244009786973	0.7435610668871516	0.0000000000000000
0.7435610668871516	0.9795244009786973	0.5000000000000000
0.2564389031128460	0.0204755990213025	0.5000000000000000
0.9795244009786973	0.2564389031128460	0.5000000000000000
0.0204755990213025	0.7435610668871516	0.5000000000000000
0.7564389331128484	0.4795244009786976	0.5000000000000000
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0.5204755990213027	0.7564389331128484	0.5000000000000000
0.4795244009786976	0.2435610968871541	0.5000000000000000
0.2435610968871541	0.4795244009786976	-0.0000000000000000
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0.4795244009786976	0.7564389331128484	-0.0000000000000000
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0.7596477099201898	0.3556164640975764	0.0000000000000000
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0.2596477099201897	0.8556164640975762	0.5000000000000000
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0.8960793605842065	0.2581387658167173	0.5000000000000000
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0.7418612341832824	0.1039206394157938	-0.0000000000000000
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0.6039206394157935	0.7581387658167176	0.5000000000000000

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0.7316836684831475	0.7683162725168583	0.0000000000000000
0.2683163315168525	0.2316837274831417	-0.0000000000000000
0.2316837274831417	0.2683163315168525	0.5000000000000000
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0.2683163315168525	0.7683162725168583	0.5000000000000000
0.7316836684831475	0.2316837274831417	0.5000000000000000