Supporting Information

$Li_3V_2(PO_4)_3$ particles embedded in N and S Co-doped porous carbon cathode for high-performance lithium storage: An experimental and DFT study

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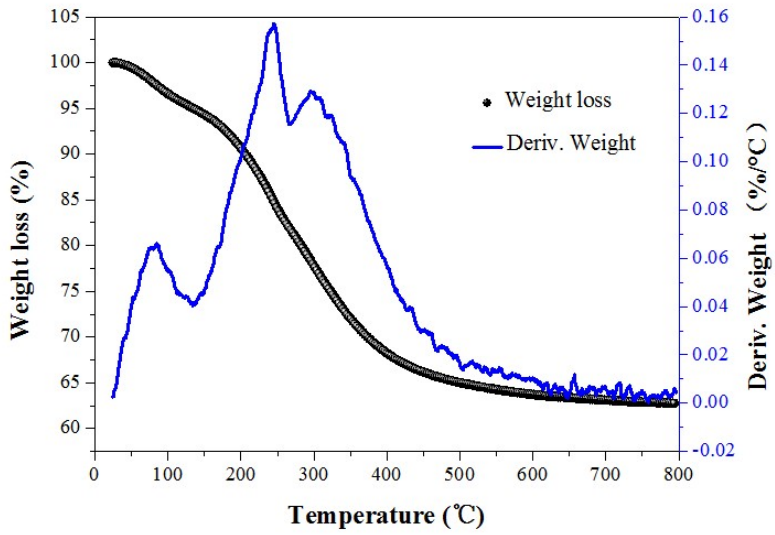

Fig. S1 TGA curve of LVP@C-NS12 was recorded under Ar atmosphere from 300 K to 1075 K.

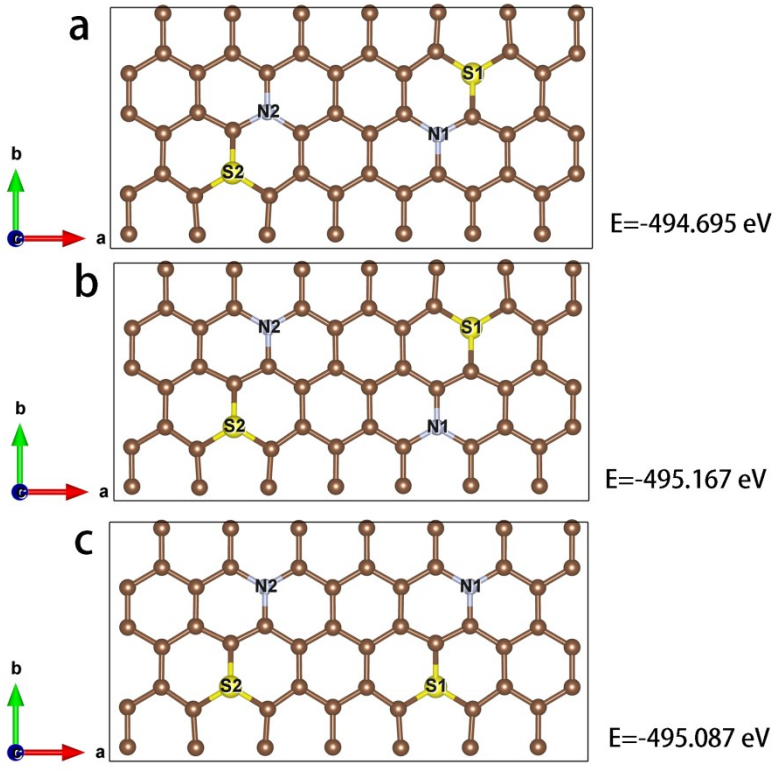

Fig. S2 Schematic illustration for the relaxed configurations of relaxed N,S co-doped C surface and its corresponding total energy：(a) coupled N and S, (b) isolated N and S type Ⅰ, (c) isolated N and S type Ⅱ co-doped carbon, respectively. The isolated N and S type Ⅰ co-doped carbon shows the lowest total energy, which represents the most thermodynamically stable configuration.

The gray ball represents carbon.

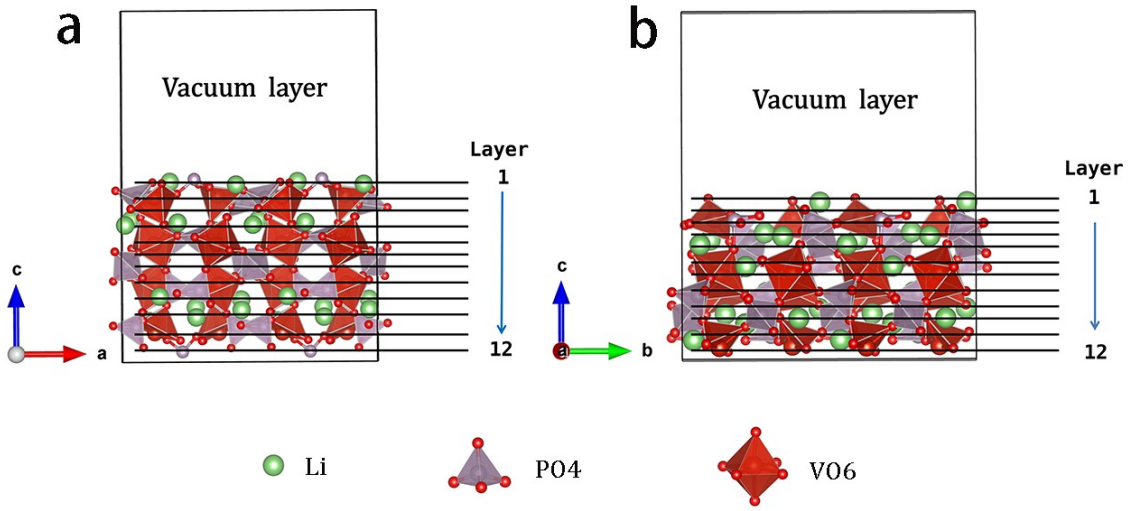

Fig. S3 Structural diagram of relaxed (2×1×1) clean surface：(a) LVP（001）surface; (b) LVP（010）surface.

Table S1 Calculated the surface energies(γ_s) results of the two surfaces of LVP at the PBE level.

Surface	$E_s^{unrelax}$（eV）	$E_s^{unrelax}$（eV）	γ_s (eV/ Å^2)
$Li_3V_2(PO_4)_3$（010）	-1037.38862	-1034.95809	0.158339
$Li_3V_2(PO_4)_3$（001）	-1055.22511	-1059.12483	0.119695

The surface energy γ_s which describes the stability of a surface, is the energy required to cleave a surface from a bulk crystal. It can be calculated by the formula according to previous literature[1]：

$$\gamma_s = \frac{1}{2A}(E_s^{unrelax} - NE_b) + \frac{1}{A}(E_s^{relax} - E_s^{unrelax})$$

Where, A is the area of the surface considered, $E_s^{unrelax}$ and E_s^{relax} is the energies of the unrelaxed and relaxed surfaces, respectively, N is the number of atoms in the slab and E_b is the bulk energy per atom.

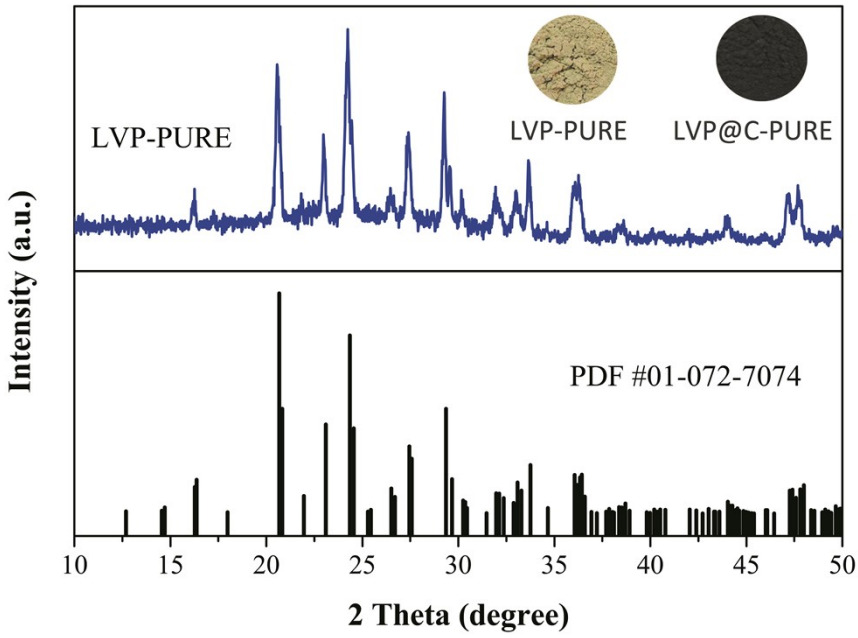

Fig. S4 XRD pattern of as prepared LVP@PURE sample.

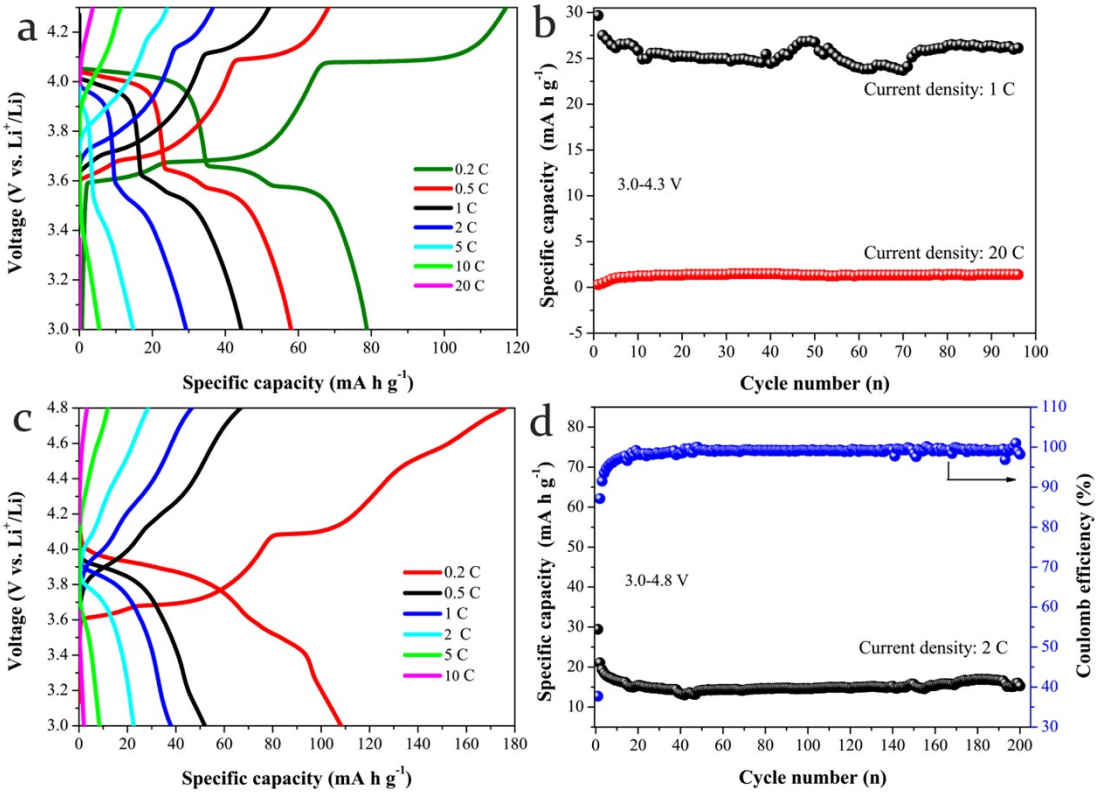

Fig. S5 GCD curves of LVP-PURE electrode at various current densities (a) and cyclic performance test at 2 C and 20 C rates (b) in a potential window of 3 - 4.3 V (vs. Li^+/Li, 1 C = 133 mAh g^{-1}); GCD curves of LVP-PURE electrode at various current densities (c) and cyclic performance test at 2 C rate (d) in the voltage range from 3 to 4.8 V (vs. Li^+/Li, 1 C = 197 mAh g^{-1}).

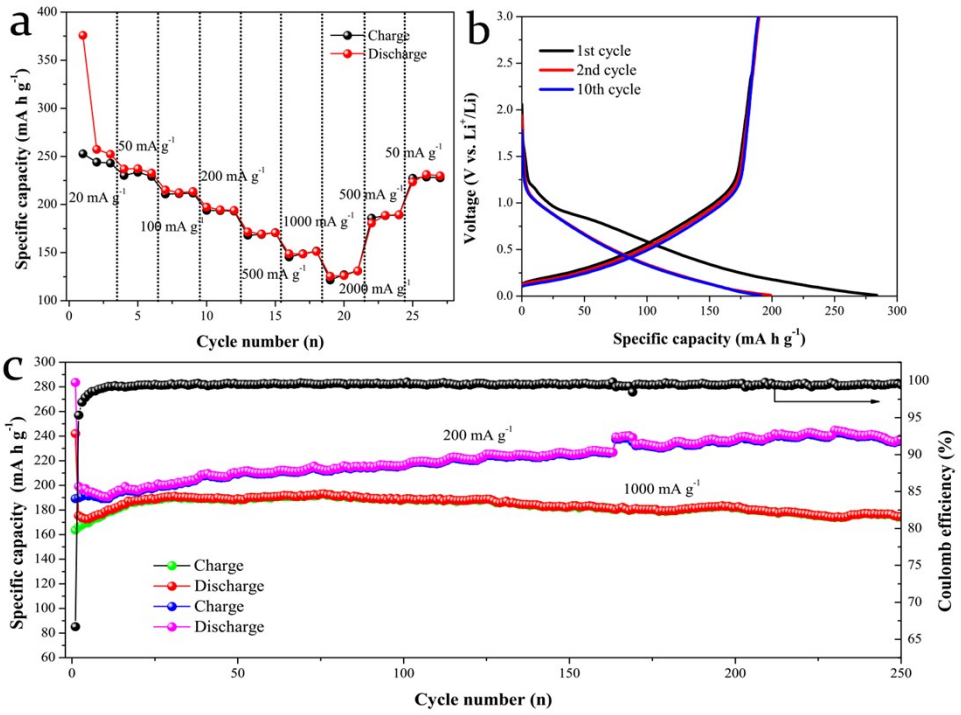

Fig. S6 (a).Rate performance of the commercial biomass hard carbon at different current densities. (b) GCD curves for 1st, 2nd and 10th at a current density of 200 mA g^{-1}. (c) Cyclic performance test at current densities of 200 and 1000 mA g^{-1} in a potential window of 0.01 - 3 V (vs. Li^+/Li).

Table S2 Comparsion of specific capacities in this work to previous LVP@C-based cathode materials. (Note: NA-The value was not given in the paper.)

Samples	Initial capicities ($mAhg^{-1}$)	Reversible capacities ($mAhg^{-1}$)	Current density (mA g^{-1})	Cycles number (n)	Voltage window (V)	DFT calculations	References
LVP@C-NS12	123.82	117.42	133	100	3-4.3	Yes	This work
LVP@C-NS12	108.83	100.22	2660	500	3-4.3	Yes	This work
LVP@C-NS12	161.13	118.22	394	200	3-4.8	Yes	This work
LVP@ S doped C	146.1	116.0	197	100	3-4.8	No	[2]
LVP@N doped C	NA	79.8	1330	600	3-4.3	No	[3]
LVP@N doped G/C	97.1	101.3	2800	500	3-4.5	No	[4]
LVP-$Na_{0.04}$@C	109.7	83.95	2660	1000	3-4.3	No	[5]
LVP@C/NCF	107.6	102.5	1330	1000	3-4.3	No	[6]
LVP@Dual Phase C	168.2	134	197	100	3-4.8	No	[7]
LVP-particle/fiber	121.09	119.55	133	500	3-4.3	No	[8]
LVP@C-fiber	149.92	107.69	197	500	3-4.8	No	[8]
LVP-$Cu_{0.05}$@C	NA	105.4	2660	200	3-4.3	No	[9]
LVP@MWCNTs/C	112.9	91.67	1995	300	3-4.3	No	[10]
LVP-$Pd_{0.05}$@C	111.9	93.78	665	150	3-4.3	No	[11]
LVP@C/3%CNT	98.7	96.1	1330	500	3-4.2	No	[12]
LVP/C-nf	94.11	72.72	133	500	3-4.3	No	[13]

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