Electronic Supplementary Material (ESI) for CrystEngComm.

Supplementary Information

Controllable Synthesis of Various V_2O_5 Micro-/Nanostructures as High Performance Cathode for Lithium Ion Batteries

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00-041-1426

Status Primary **QM:** Star **Pressure/Temperature:** Ambient **Chemical Formula:** V2 O5
Empirical Formula: O5 V2 **Weight %:** O43.98 V56.02 **Atomic %:** O71.43 V28.57
Compound Name: Vanadium Oxide **Mineral Name:** Shcherbinaite, syn

Radiation: CuKá : 1.5418 Å **Filter:** Graph Mono **d-Spacing:** Diff. **Cutoff:** 15.00 **Intensity:** Diffractometer
I/Ic: 1.6

SYS: Orthorhombic **SPGR:** Pmmn (59)
Author's Cell [AuthCell a: 11.516(4) Å **AuthCell b:** 3.5656(4) Å **AuthCell c:** 4.3727(4) Å
AuthCell Vol: 179.55 Å³ **AuthCell Z:** 2.00 **AuthCell MolVol:** 89.78]
Author's Cell Axial Ratio [c/a: 0.380 **a/b:** 3.230 **c/b:** 1.226]
Density [Dcalc: 3.364 g/cm³ **Dmeas:** 3.32 g/cm³] **SS/FOM:** F(30) = 92.1(0.0096, 34)
Temp: 298.000 K (Ambient temperature assigned by ICDD editor) **Color:** Dark orange

Space Group: Pnmm (59) **Molecular Weight:** 181.88
Crystal Data [XtlCell a: 4.373 Å **XtlCell b:** 11.516 Å **XtlCell c:** 3.566 Å **XtlCell :** 90.00° **XtlCell :** 90.00°
XtlCell : 90.00° **XtlCell Vol:** 179.55 Å³ **XtlCell Z:** 2.00]
Crystal Data Axial Ratio [c/a: 0.815 **a/b:** 0.380 **c/b:** 0.310]
Reduced Cell [RedCell a: 3.566 Å **RedCell b:** 4.373 Å **RedCell c:** 11.516 Å **RedCell :** 90.00°
RedCell : 90.00° **RedCell :** 90.00° **RedCell Vol:** 179.55 Å³]

: =2.25 calc

Atomic parameters are cross-referenced from PDF entry 04-007-0398 **ADP Type:** B **Origin:** O2
Crystal (Symmetry Allowed): Centrosymmetric

SG Symmetry Operators:

Seq	Operator	Seq	Operator	Seq	Operator	Seq	Operator
1	x,y,z	3	-x+1/2,y,z	5	x,-y+1/2,z	7	-x+1/2,-y+1/2,z
2	-x,-y,-z	4	x+1/2,-y,-z	6	-x,y+1/2,-z	8	x+1/2,y+1/2,-z

Atomic Coordinates:

Atom	Num	Wyckoff	Symmetry	x	y	z	SOF	Biso	AET
V	1	4f	.m.	0.10118	0.25	0.8917	1.0	0.54	5-a
O	2	4f	.m.	0.1043	0.25	0.531	1.0	1.21	1#a
O	3	4f	.m.	-0.0689	0.25	0.003	1.0	0.79	3#a
O	4	2a	mm2	0.25	0.25	0.001	1.0	0.9	2#a

Fig. S1 ICSD data of V_2O_5.

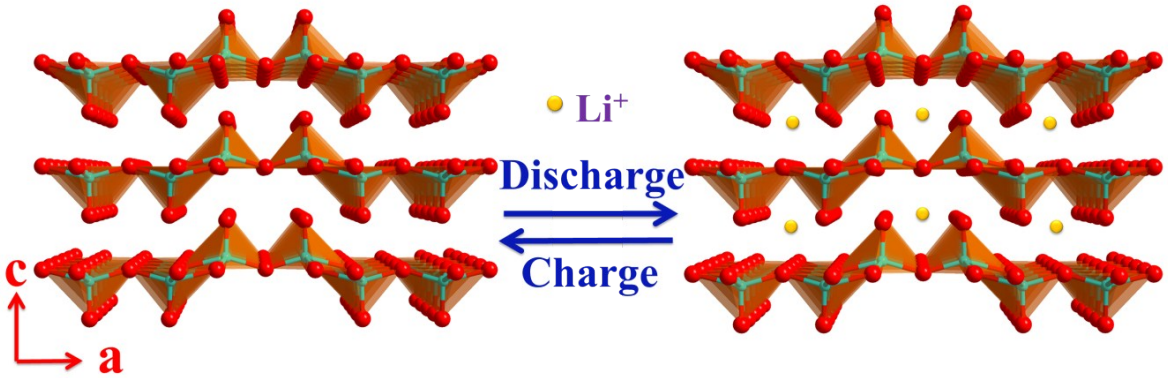

Fig. S2 Schematic illustration showing fast Li^+ transportation along the a-b plane of layered V_2O_5 structure.

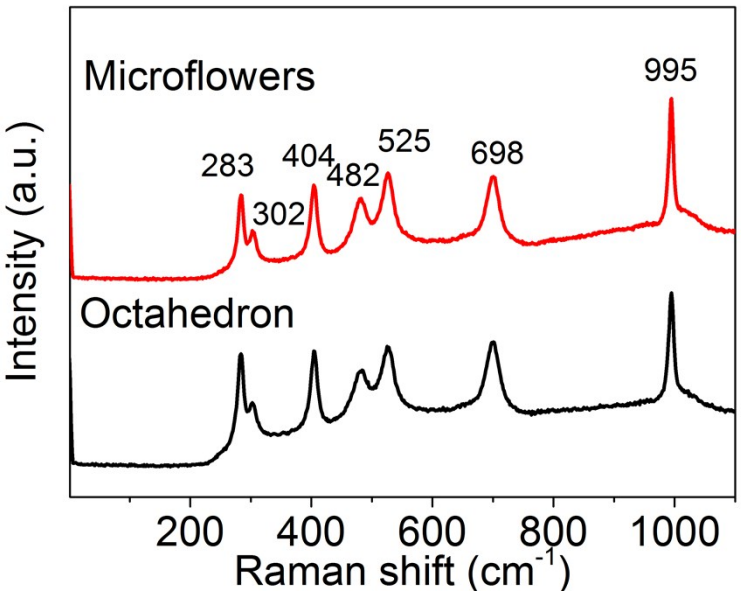

Fig. S3 Raman spectra of the V_2O_5 microflowers and octahedrons.

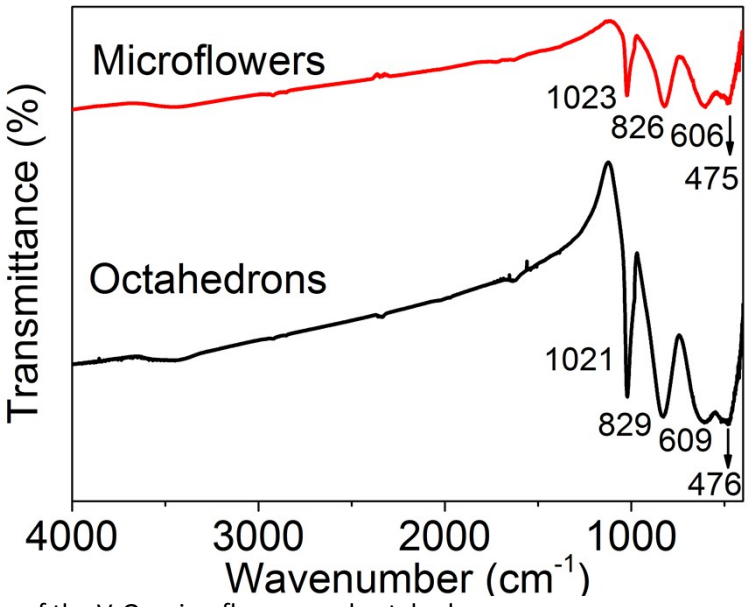

Fig. S4 FTIR spectra of the V_2O_5 microflowers and octahedrons.