Electronic Supplementary Material (ESI) for RSC Advances.

Surporting information

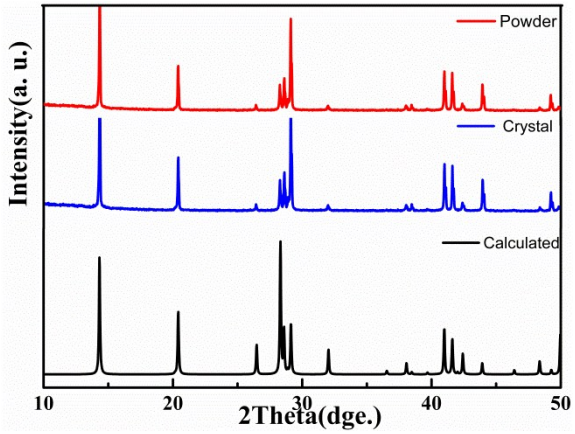

Fig. S1 Experimental and calculated powder X-ray diffraction patterns for polycrystalline and crystal $LiVMoO_6$

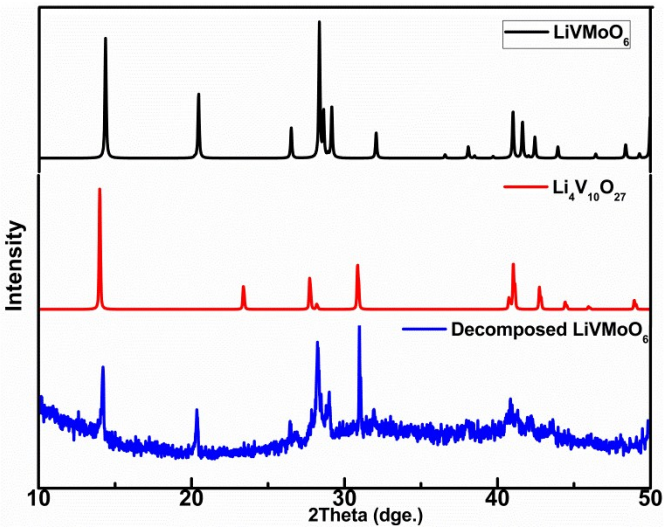

Fig. S2 Powder X-ray diffraction patterns for decomposed crystal $LiVMoO_6$.

Table S1 Crystal data and structure refinement for monoclinic $LiVMoO_6$

Empirical formula	$LiVMoO_6$
Formula weight/g·mol-1	249.82
Temperature/K	296(2)
Wavelength/Å	0.71073
Crystal system, space group	Monoclinic, *C*2/m
Unit cell dimensions/Å	*a*=9.3531(9), *b*=3.6477(4), *c*=6.647(7) b=3.6477(4) *α*(deg)=90° *β*(deg)=111.6430°
Volume (Å3)	210.79
Z	2
T(K)	296
Absorption coefficient, μ(mm-1)	4.967
Theta range for data collection (°)	3.3 to 22.52
Limiting indices	$-12 \le h \le 12$, $-4 \le k \le 4$, $-8 \le l \le 8$
R(int)	0.0139
Independent reflection	1251
Absorption correction	Semi-empirical from equivalent
Refinement method	Full-matrix least-squares on F2
Goodness-of-fit on F^2	1.229
Final R indices $[I > 2\sigma(I)]$[a]	R_1=0.0138，wR_2=0.0334
R indices (all data)	R_1=0.0123，wR_2=0.0332
Extinction coefficient	0.0179(16)
largest diff. peak and hole ($e \cdot A^{-3}$)	0.190 and -0.207

[a] $R_1 = \sum ||F_o| - |F_c|| / \sum |F_o|$, $wR2 = \{\sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2]\}^{1/2}$

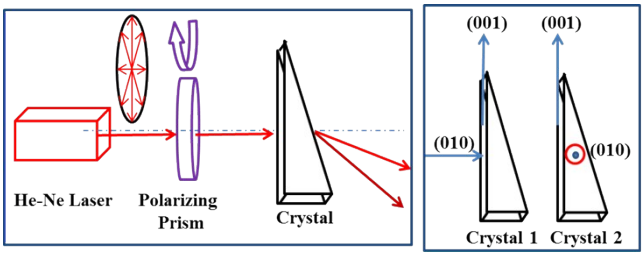

Fig. S3 Schematic of the experimental facilities to determined optical principle axes

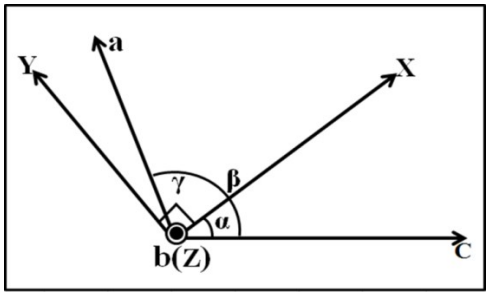

Fig. S4 Relative orientation of the optical axes (*X*, *Y*, and *Z*) with regard to the crystallographic axes (*a*, *b*, and *c*) for the monoclinic $LiVMoO_6$ single crystals, α=40º, β=111º, γ=90º

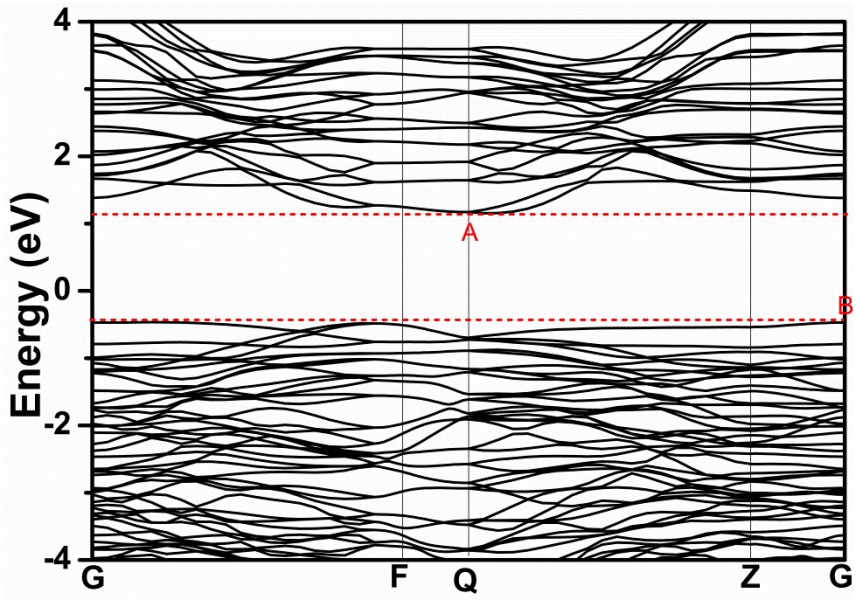

Fig. S5 The band structure of $LiVMoO_6$ near fermi level. The lowest CB and the highest VB located at “A” and “B” respectively.