

Electronic Supplementary Information

Probing Lattice Vibration and Surface Electronic State in Layered (NH₄)₂V₃O₈ Single Crystal

Haiping Chen,^a Zhongti Sun,^b Chengming Wang,^c Xiuling Li,^b Xusheng Zheng,^a Youkui Zhang,^a Qun He,^a
Xiaojun Wu,^{*b} and Li Song^{*a}

* song2012@ustc.edu.cn (L. Song); xjwu@ustc.edu.cn (X.J. Wu)

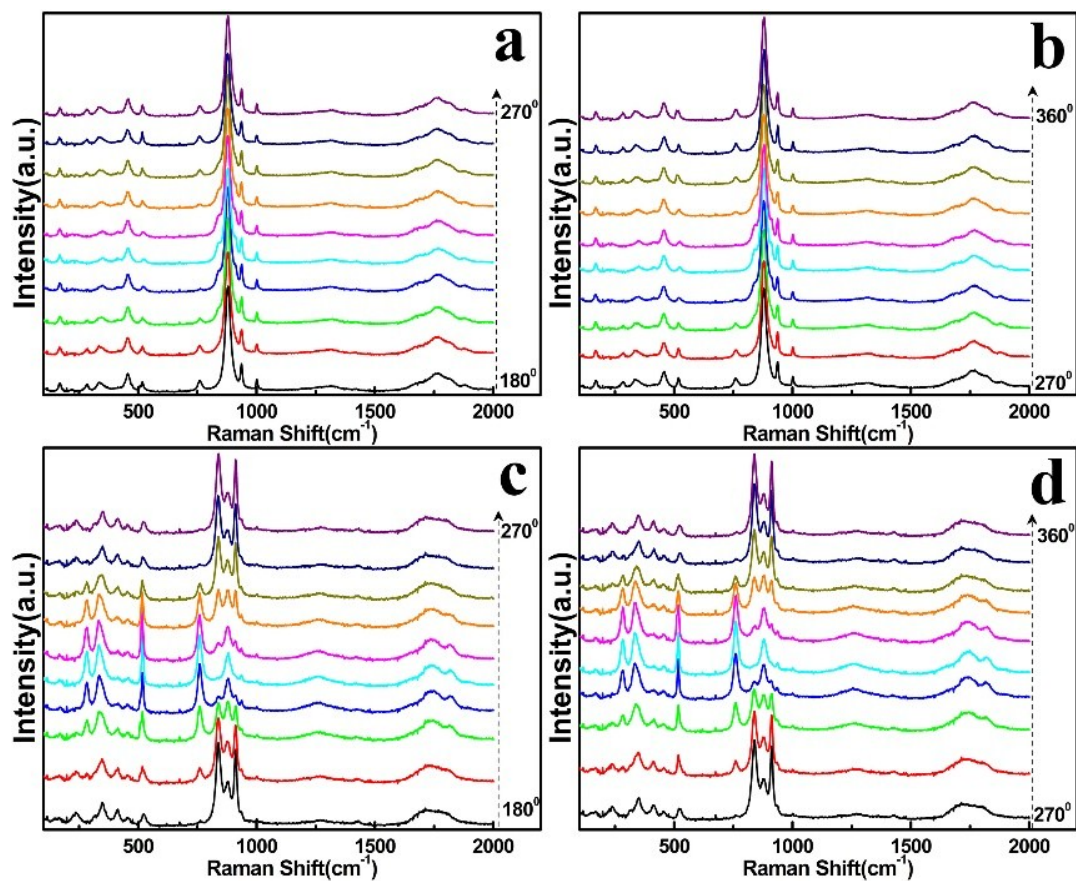


Fig. S1. The angle dependence of Raman peak intensity from 180° to 360°, (a) and (b) parallel polarization Z(XX)Z, (c) and (d) vertical polarization Z(ZX)Z.

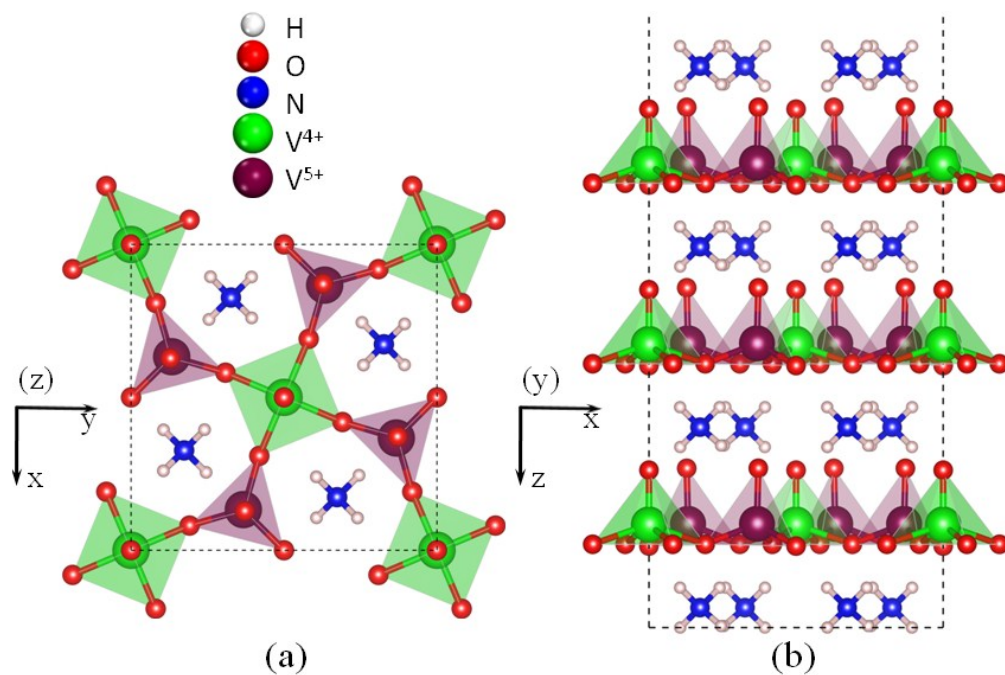


Fig. S2 (a) Viewed from *c* axis, (b) viewed from *b* axis.

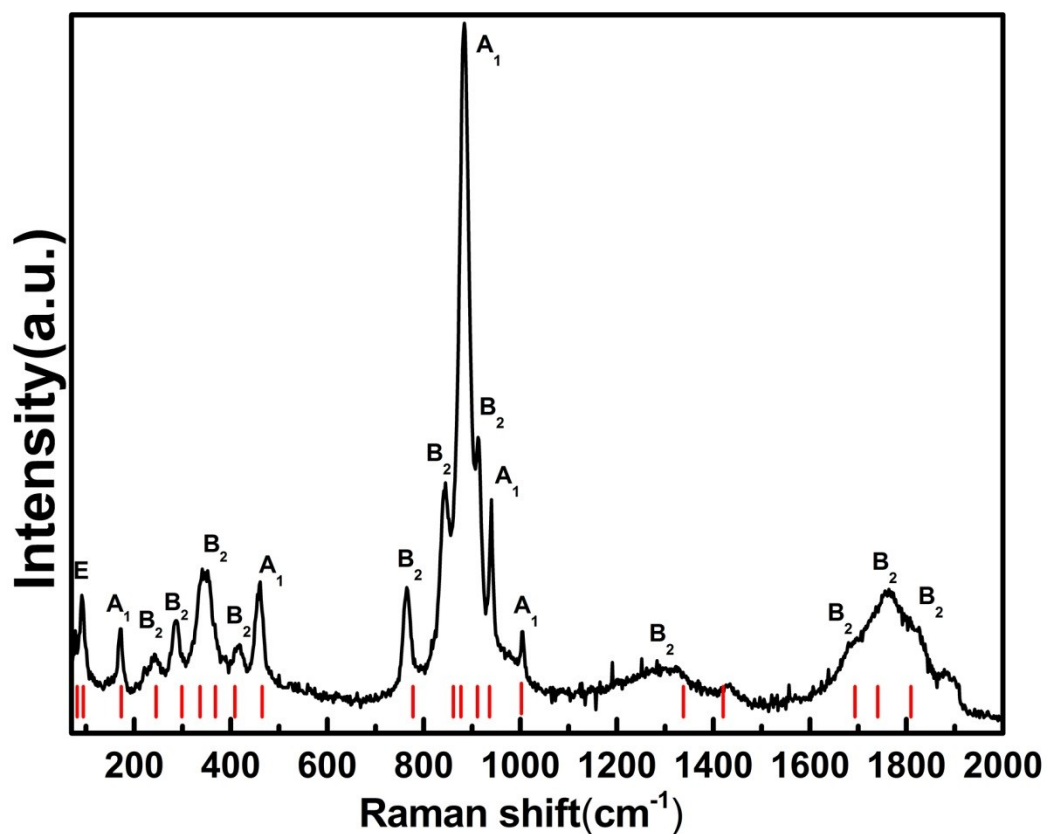


Fig. S3. The comparison of experimental Raman peaks with the calculated phonon frequency at Γ k-point (marked as red lines) for $(\text{NH}_4)_2\text{V}_3\text{O}_8$.

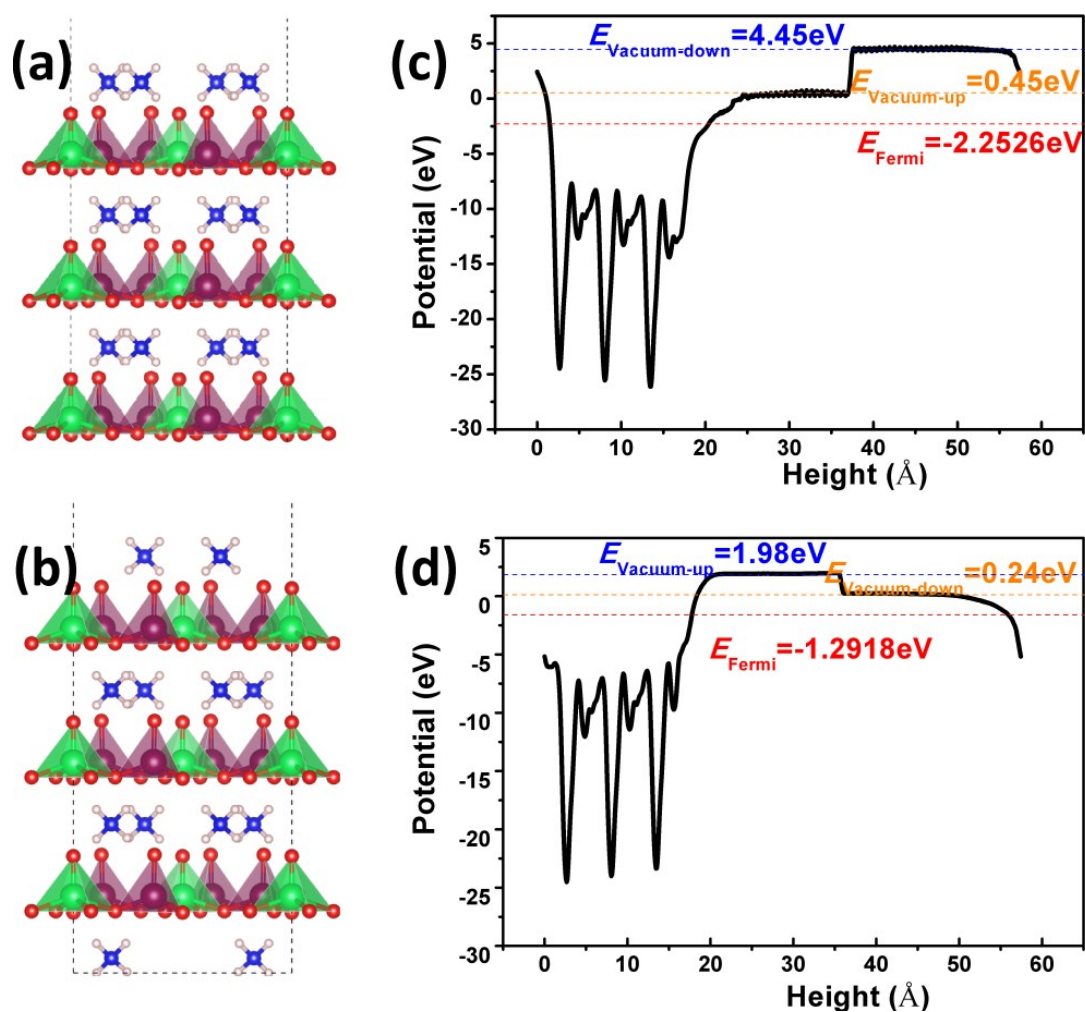


Fig. S4. The structures of (001) surface of $(\text{NH}_4)_2\text{V}_3\text{O}_8$ with (a) NH_4^+ ions and $\text{V}_3\text{O}_8^{2-}$ surface, and (b) NH_4^+ ions surface with with half number of NH_4^+ ions removed. (c) and (d) are the corresponding potential profiles, (d) is the optimized potential.