

Supplementary Information

Electronic and vibrational decoupling in chemically exfoliated bilayer 2D-V₂O₅

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The Raman spectrum collected for sample S2 is fitted using Gaussian- Lorentzian mixed function for the range 100-800 cm⁻¹ as shown in Figure S-1. The fitted spectrum consists of the Raman modes at 111, 162, 267, 324, 493, 539, 619 and 711 cm⁻¹. The asymmetric mode at 1010 cm⁻¹ is fitted using the Breit–Wigner–Fano (BWF) line shape function. The Fano type asymmetry can appear because of the charge doping due to the presence of oxygen vacancy defects. Similar asymmetric broadening in Raman modes is observed in hole doped graphene [1,2].

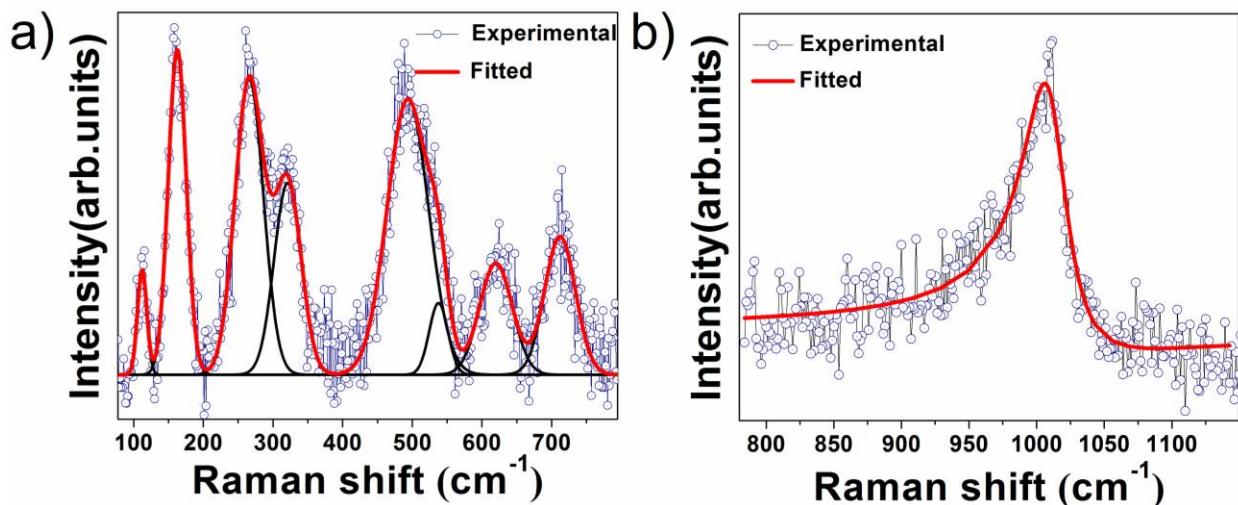


Figure S-1 a) Raman spectrum with mixed Gaussian– Lorentzian profile fit for the 100-800 cm⁻¹ spectral range. b) Asymmetric peak at 1010 cm⁻¹, fitted with Breit–Wigner–Fano (BWF) line shape function in the 800-1200 cm⁻¹ spectral range.

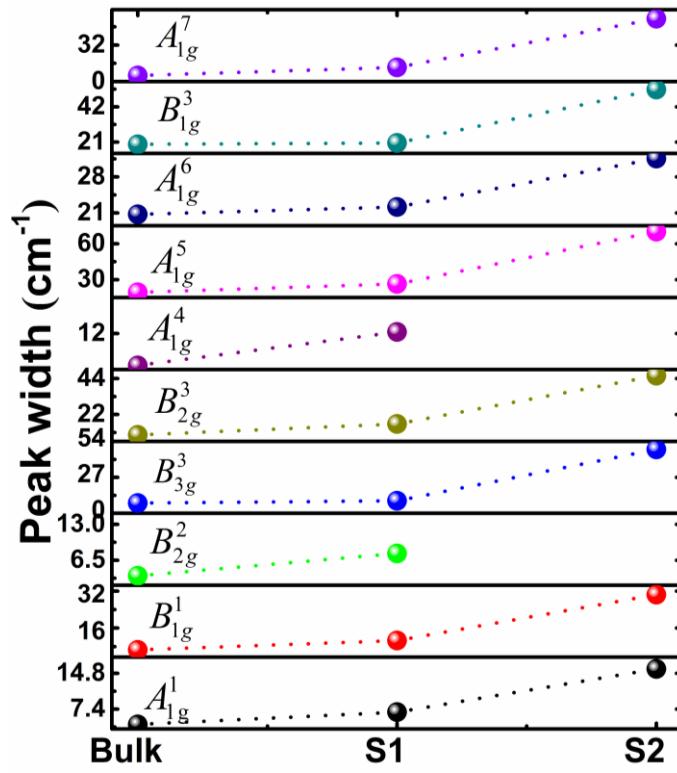


Figure S-2 Line width (FWHM) of peaks in Raman spectra of bulk and the exfoliated samples S1 and S2.
Dotted lines are a guide to the eyes.

V_2O_5 is having layers stacked along (001) direction. As mentioned earlier, the value of lattice parameter c in α - polymorph of orthorhombic V_2O_5 is 0.43 nm. The unit cell of $\alpha\text{-V}_2\text{O}_5$ consists of two VO_5 square pyramidal units, which are extended along the b - axis through O_{II} and along the a -axis through O_{III} to form the monolayer along ab -plane. It means that the thickness of a monolayer 2D- V_2O_5 can be estimated as the sum of bond length of the $\text{V-O}_1 \pi$ -bond and the van der Waals bond between them as shown in Figure S-3. The thicknesses of monolayer, bilayer, trilayer and quad-layer 2D- V_2O_5 are calculated as 0.43, 0.87, 1.3 and 1.74 nm, respectively.

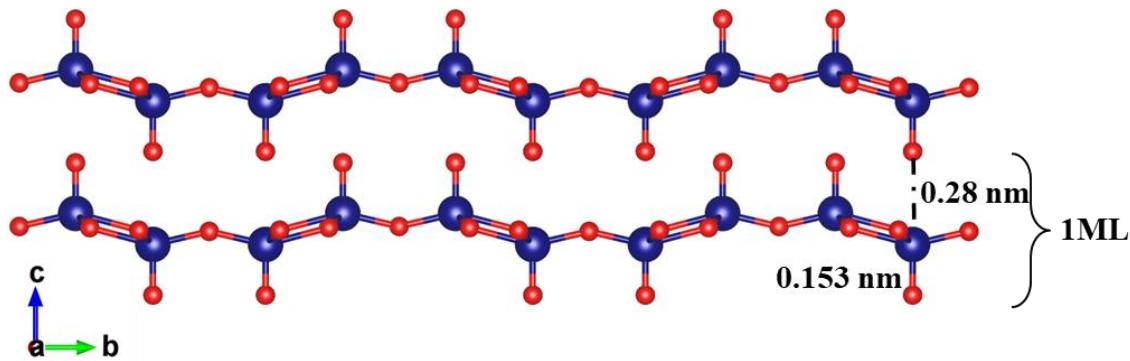


Figure S-3 Schematic diagram of the structure of V_2O_5 . The thickness of one monolayer shown in the figure as the sum of bond lengths of $\text{V}=\text{O}_1$ and the van der Waals bond, i.e 0.43 nm.

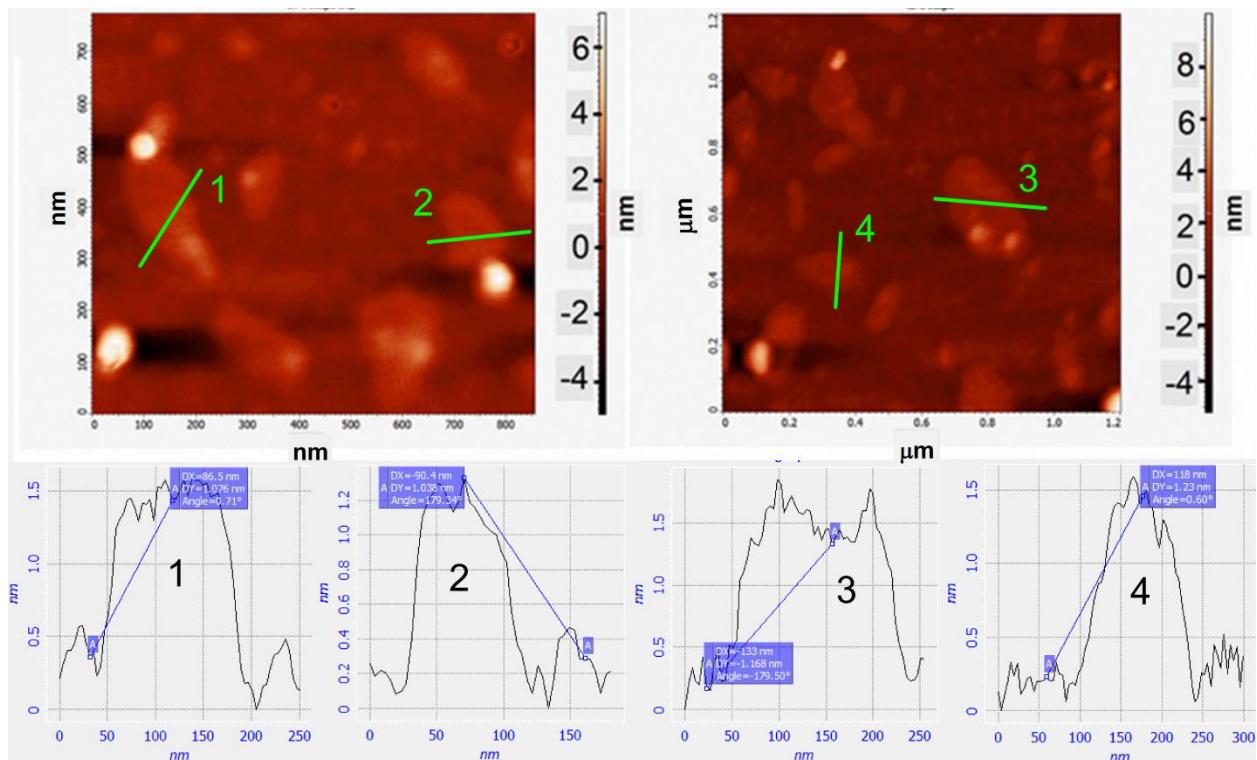


Figure S-4 a) AFM images of exfoliated V_2O_5 nanosheets (S2). The line profile of height for the marked regions are also shown in the figure. Thicknesses of the nanosheets marked as 1,2,3 and 4 are 1.07, 1.03, 1.16 and 1.2 nm, respectively.

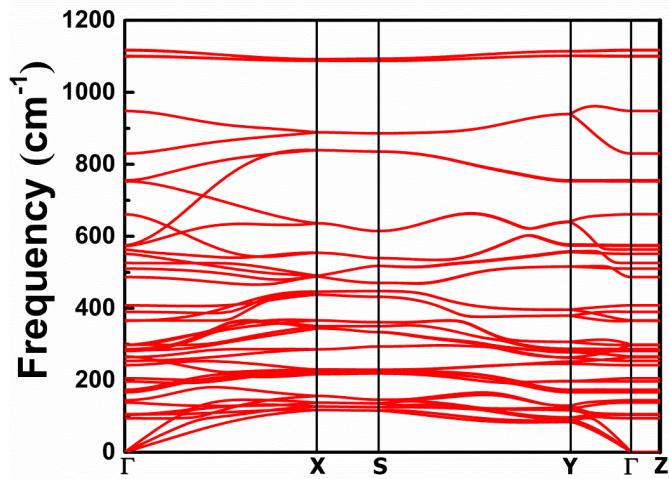


Figure S-5. Phonon dispersion curve for monolayer 2D-V₂O₅.

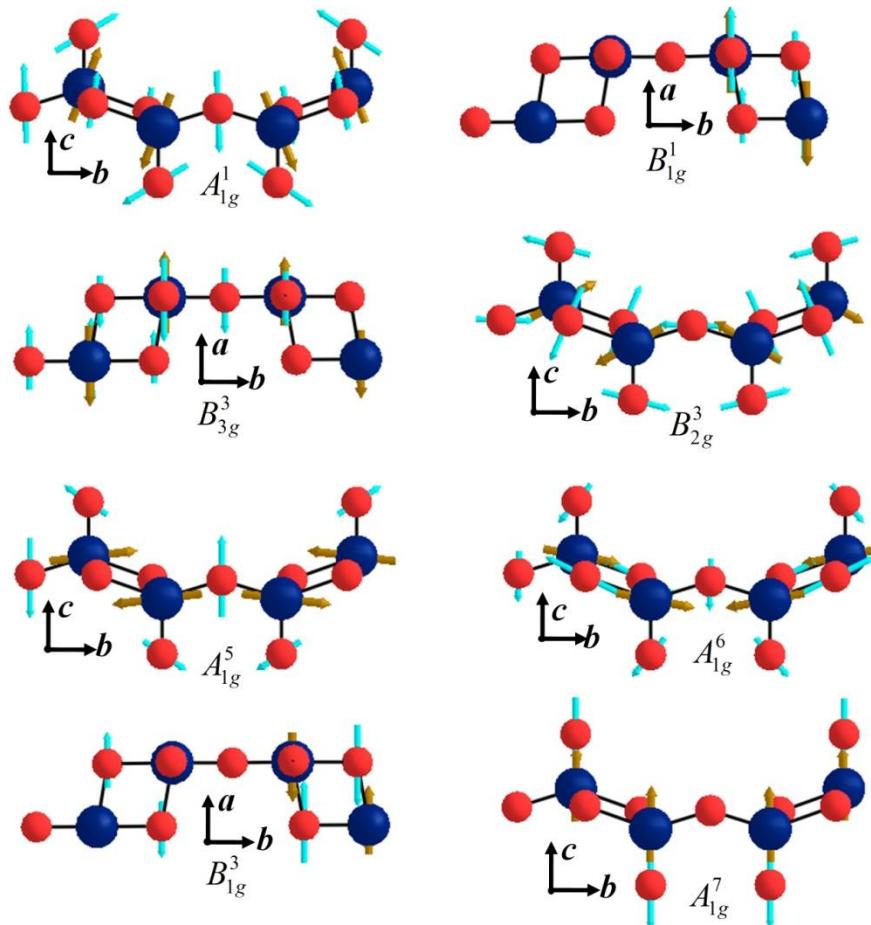


Figure S-6 Polarization of Raman active vibrational modes of monolayer 2D-V₂O₅.

Polarization of experimentally observed Raman modes of 2D V₂O₅ is shown in Figure S-6. The low frequency vibrational modes A_{1g}^1 and B_{1g}^1 are due to the chain translation along c and a -axes.

In A_{1g}^1 mode, the bridge oxygen vibrates in the c direction, as a result, the entire chain on both sides of O_{II} moves up and down with O_{II}. In B_{1g}^1 mode, V atoms move back and forth in a direction and this motion ends up with the stretching vibration of V–O_{III} along a -axis and a deflection of V–O_I along a direction. The mode B_{3g}^3 is due to V–O_{II}–V bending and deflection of V–O_I along a direction. The stretching caused by the deflection of V–O_{III} and V–O_{III'} along c direction and V–O_I deflection in b direction causes for the vibrational mode B_{2g}^3 . A_{1g}^5 mode arises from the bending of V–O_{II}–V in c direction and stretching of V–O_{III'} along b direction. A_{1g}^6 mode is due to the stretching vibration of V–O_{III'} and V–O_{III} along with V–O_{II}–V bending. The deflection of V–O_{III'} and V–O_{III} along a direction originates the vibrational mode B_{1g}^3 . The highest frequency mode A_{1g}^7 corresponds to the stretching vibration of V–O_I along c -axis.

References

- 1 Tang, T.-T., et al., A tunable phonon–exciton Fano system in bilayer graphene. *Nature Nanotechnology*, **5**, 32-36(2010).
- 2 Yoon, D., et al., Fano resonance in Raman scattering of graphene. *Carbon*, **61**, 373-378(2013).