

Electronic Supplementary Information

Ultrafast carrier dynamics in vanadium doped MoS₂ alloys

Bhuvan Upadhyay^{1,2}, Rahul Sharma^{3,4}, Dipak Maity³, Tharangattu N. Narayan³, Suman Kalyan Pal^{1,2}

¹School of Physical Sciences, Indian Institute of Technology Mandi, Kamand, Mandi, Himachal Pradesh, 175075, India

²Advanced Materials Research Center, Indian Institute of Technology Mandi, Kamand, Mandi, Himachal Pradesh, 175075, India

³Tata Institute of Fundamental Research-Hyderabad, Sy. No. 36/P, Gopanapally Village, Serilingampally Mandal, Hyderabad-500046, India

⁴Department of physics and Astronomy, Uppsala university, 75236, Uppsala, Sweden

Determination of the free electron density (n_f)

The value of n_f was calculated using Debye-Huckel screening length (L_{sc}) relation

$$n_f = \frac{K_p k_B T}{2e^2 L_{sc}}$$

considering the parameter values $L_{sc} = a_B = 0.6 \text{ nm}^1$, $K_p = \epsilon \times \epsilon_0 = 2.85 \times 8.54 \times 10^{-12} \text{ C}^2/\text{N}\cdot\text{m}^2$, $e = 1.6 \times 10^{-19} \text{ C}$, $T = 300 \text{ K}$, and $k_B = 1.38 \times 10^{-23} \text{ J/K}$.

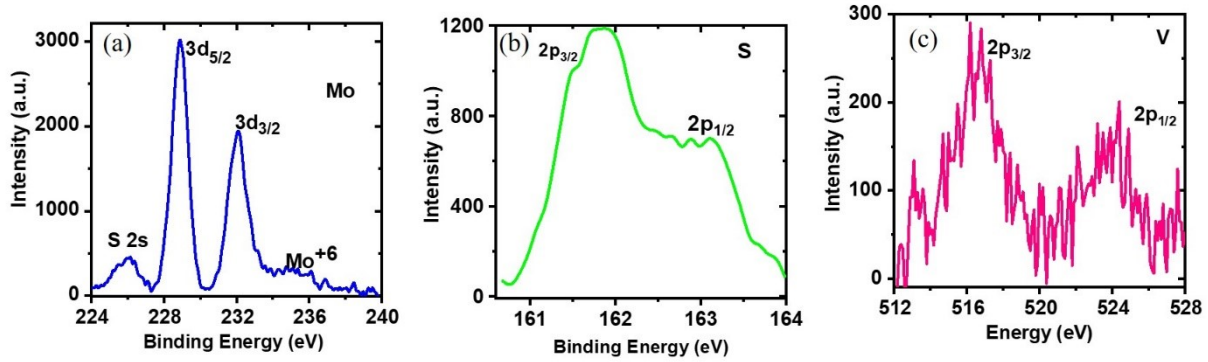


Fig. S1 X-ray photoemission spectra (XPS) of MH-V-MoS₂ corresponding to (c) molybdenum (Mo), (d) sulphur (S) and (e) vanadium (V).

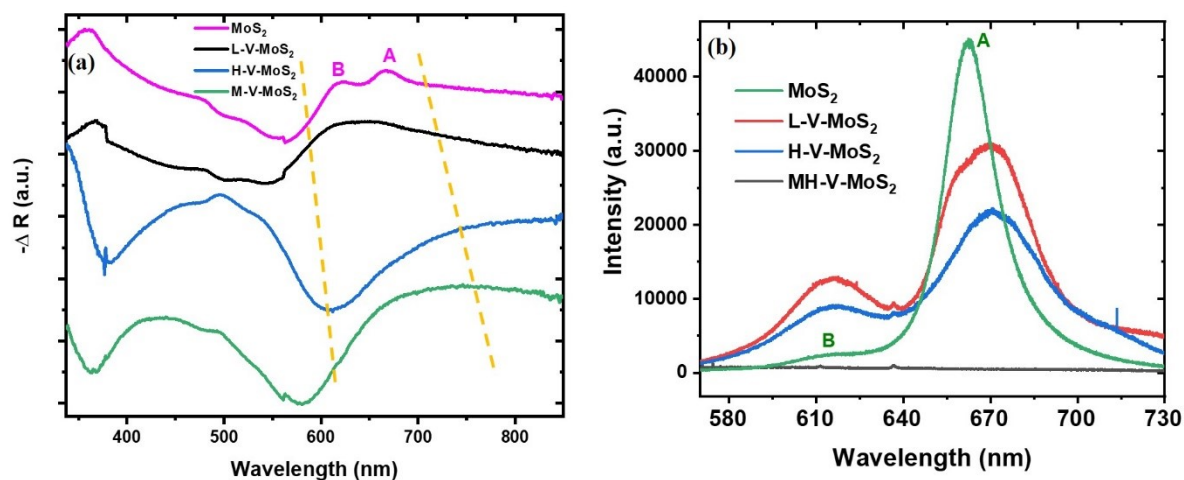


Fig. S2 (a) Linear reflection spectra and (b) photoluminescence (PL) spectra of pristine and V-doped MoS₂ samples.

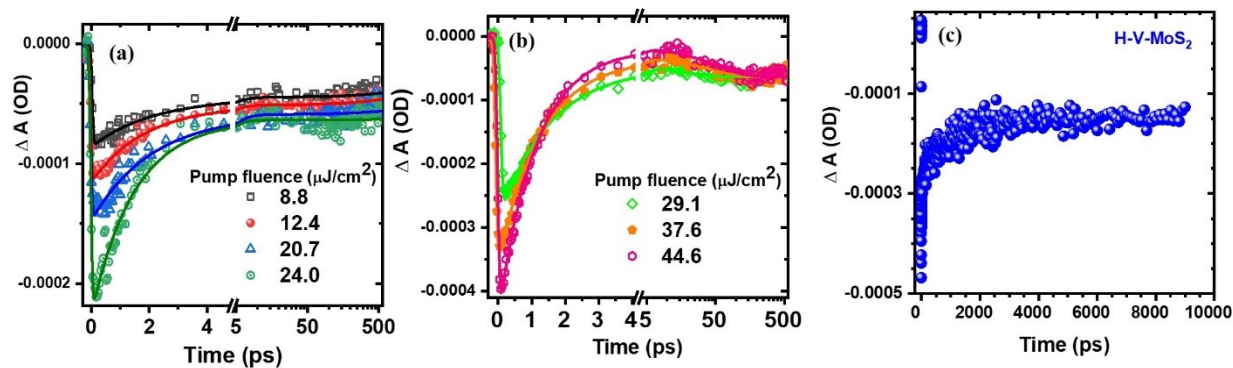


Fig. S3 (a-b) Fitting results for TA kinetics measured at different pump fluences in H-V-MoS₂. Pump and probe wavelengths used during measurements were 480 and 660 nm, respectively. (c) TA kinetics of H-V-MoS₂ measured up to 9 ns with 660 nm probe and 480 nm pump lights.

Table S1. Atomic percentage of Mo, V and S in H-V-MoS₂ alloy obtained from XPS spectra.

Element- orbital	Peak BE (eV)	FWHM (eV)	Area (P) CPS.eV	Atomic %
S-2p	162.12	1.09	7706.58	64.29
Mo-3d	229.16	1.12	21630.97	32.09
V-2p	513.58	1.08	1691.38	3.62

Table S2. Atomic percentage of Mo, V and S in MH-V-MoS₂ alloy obtained through XPS measurements.

Element -orbital	Peak BE (eV)	FWHM (eV)	Area (P) CPS.eV	Atomic %
S-2p	161.89	1.16	2374.60	60.95
Mo- 3d	228.90	1.02	6941.79	31.69
V-2p	516.63	2.27	1115.12	7.36

Table S3. Fitting results of TA kinetics for A-exciton of ML MoS₂ measured with different pump energy.

Pump energy (eV)	τ_1 ps (A ₁ %)	τ_2 ps (A ₂ %)	τ_3^* ps (A ₃ %)
3.02	0.20±0.01 (73)	7.50±0.69 (19)	500 (8)
2.58	0.19±0.01 (71)	8.00±0.57 (15)	500 (14)
2.33	0.20±0.01 (67)	7.16±0.35 (22)	500 (11)
2.00	0.21±0.01(60)	16.32±1.12 (23)	500 (17)

* The value of τ_3 was kept constant during fitting

Table S4. Fitting results of TA kinetics at A' band of L-V-MoS₂ measured with different pump energy.

Pump energy (eV)	τ_1 ps (A ₁ %)	τ_2 ps (A ₂ %)	τ_3^* ps (A ₃ %)
3.02	0.18±0.01 (56)	8.60±0.69 (21)	1000 (23)
2.58	0.25±0.02 (46)	9.50±0.91 (24)	1000 (30)
2.33	0.23 ±0.02 (37)	8.30±0.87 (25)	1000 (38)
2.00	0.25±0.09 (31)	10.69±2.09 (31)	1000 (38)

* The value of τ_3 was kept constant during fitting

Table S5. Results of the fitting of TA kinetics of H-V-MoS₂ measured at 665 nm with a pump wavelength 480 nm.

Pump fluence ($\mu\text{J}/\text{cm}^2$)	Decay-1 (ps) (#FC %)	Decay-2* (ps) (FC %)	Rise (ps) (FC %)
8.8	2.21 \pm 0.23 (83)	1000 (17)	-
12.4	1.84 \pm 0.11 (85)	1000 (15)	-
20.7	2.11 \pm 0.14 (93)	1000 (7)	-
24.0	1.49 \pm 0.07 (99)	1000 (1)	-
29.1	1.56 \pm 0.07 (100)	-	17.44 \pm 7.77 (100)
37.6	1.29 \pm 0.03 (100)	-	41.37 \pm 7.97 (100)
44.5	1.12 \pm 0.02 (100)	-	52.54 \pm 6.38 (100)

* The value of decay-2 was kept constant during fitting

#FC: fractional contribution

References

- 1 Y. Yu, G. Li and L. Cao, *arXiv*, 2020, 2007.11509.