

Supplementary Information

Interactions at heterointerfaces influence actuation in wet cast 1T-MoS₂ and V₂O₅ · 0.5 H₂O thin films

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Table of Contents

Supporting Figures and Tables.....	3
Dependence of strain on scan rate 1T-MoS ₂ Au Kapton electrode	3
Nanoindentation of 1T-MoS ₂	4
Scan rate dependance of 1T-MoS ₂ CV	5
CV scan rate dependence of 1T-MoS ₂ Ni Kapton electrode	6
Dependence of strain % on potential for multiple cycles for 1T-MoS ₂ electrodes.....	7
Dependence of actuation on scan rate for V ₂ O ₅ · 0.5 H ₂ O Au Kapton electrode.....	8
Schematic of V ₂ O ₅ · 0.5 H ₂ O Au Kapton electrode	9
FTIR spectrum of V ₂ O ₅ · 0.5 H ₂ O	10
UV- <i>vis</i> spectra of V ₂ O ₅ · 0.5 H ₂ O	11
Electrochromic behavior of V ₂ O ₅ · 0.5 H ₂ O	12
Dependence of peak current density on scan rate for V ₂ O ₅ · 0.5 H ₂ O.....	13
Chronoamperometry of a V ₂ O ₅ · 0.5 H ₂ O Au Kapton electrode.....	14
CV at different scan rates for a V ₂ O ₅ · 0.5 H ₂ O Au Kapton electrode	15
Dependence of strain % on potential for multiple cycles for V ₂ O ₅ · 0.5 H ₂ O electrodes..	16
Dependence of actuation on scan rate for a V ₂ O ₅ · 0.5 H ₂ O Au Kapton electrode	17
Dependence of strain on scan rate for a V ₂ O ₅ · 0.5 H ₂ O electrode.....	18
Nanoindentation of V ₂ O ₅ · 0.5 H ₂ O	19
Actuation metrics for V ₂ O ₅ · 0.5 H ₂ O electrodes using crystallographic strains.....	20
Actuation metrics for V ₂ O ₅ · 0.5 H ₂ O electrodes	20
Table of actuation metrics of 1T-MoS ₂ electrodes.....	20
Table of actuation metrics for reported V ₂ O ₅ based actuators	21
Table of actuation metrics for reported MoS ₂ based actuators	21

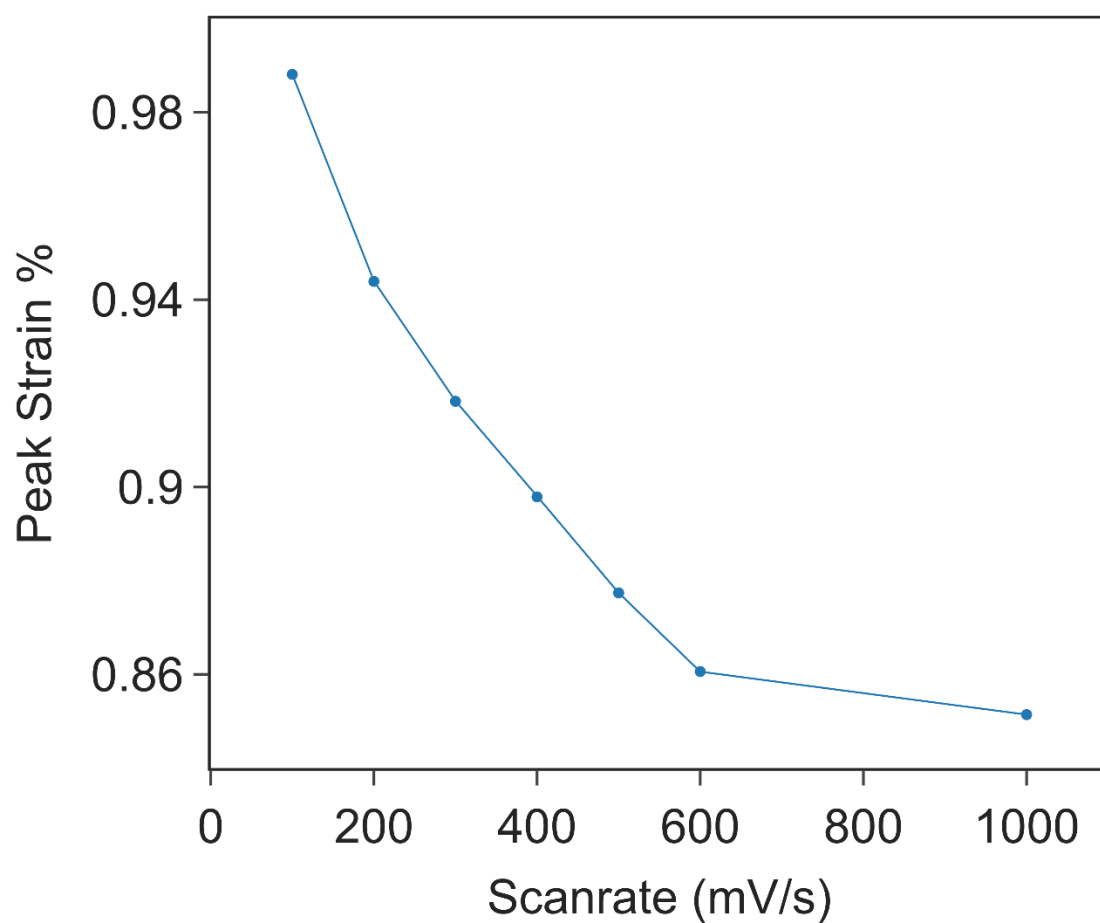


Figure S1. Peak Strain % values calculated during actuation of a 1T-MoS₂ | Au | Kapton electrode at various potential scan rates. CV was performed in 0.5 M Na₂SO₄ aqueous electrolyte with platinum wire counter and Ag/AgCl reference electrodes over a potential window of -0.3 to 0.3 V.

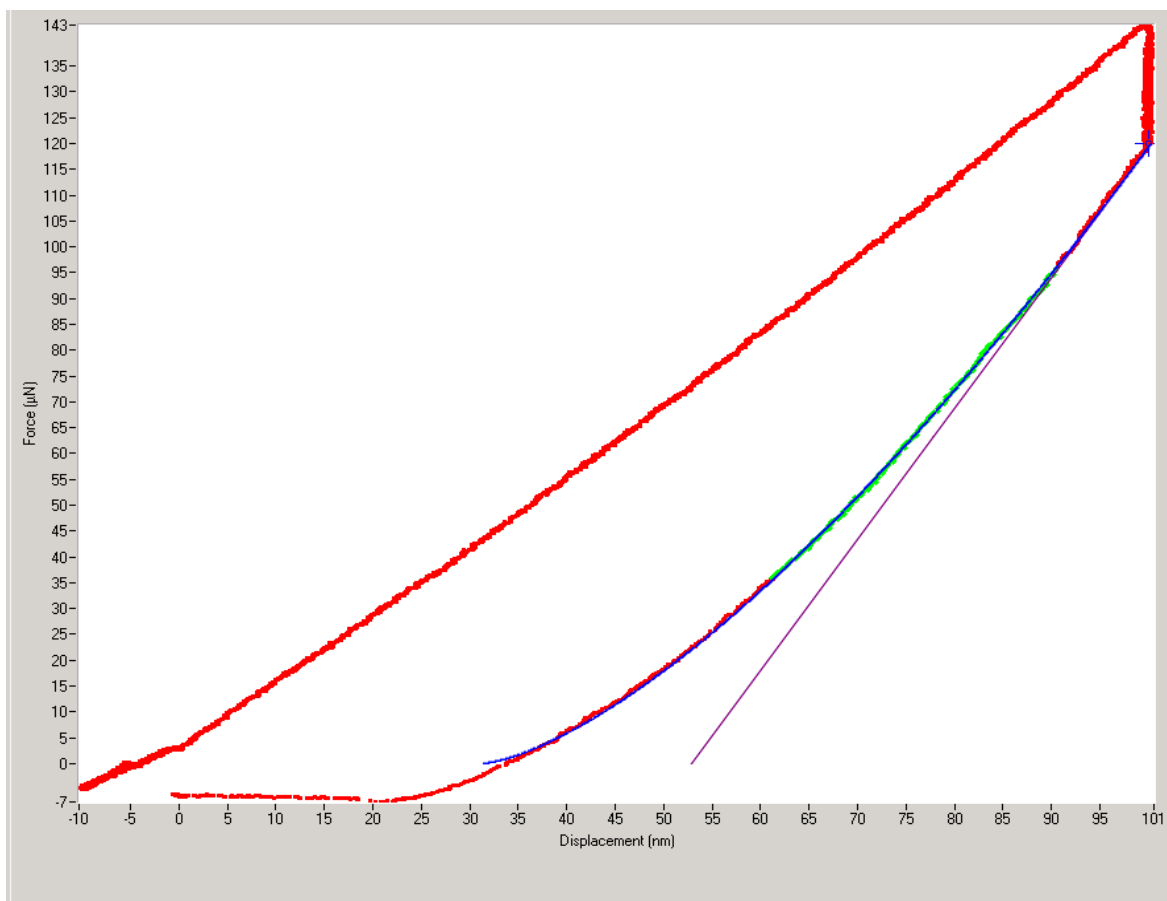


Figure S2. Nanoindentation measurement of deposited 1T-MoS₂. Indent depth was kept below ~ 10% of the active layer thickness to avoid influence from the substrate. Based on the displacement response to the applied force, an out of plane Young's modulus of 5.01 GPa and was converted to the in-plane Young's modulus using the Poisson ratio of 1T-MoS₂ (0.3) and was found to be 1.50 GPa.⁵⁴

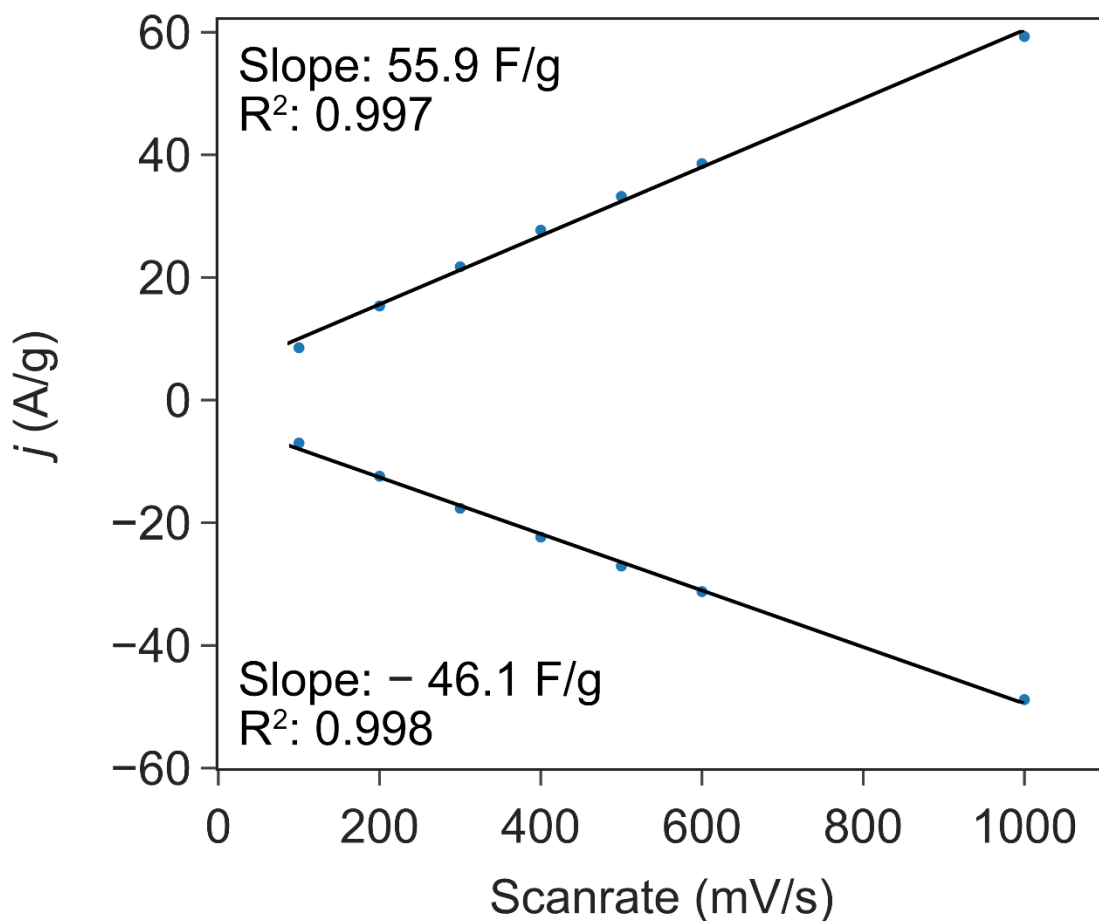


Figure S3. Charging current for a 1T-MoS₂ | Au | Kapton electrode plotted vs scan rate. The slope represents the specific capacitance in F/g for the positive and negative charging current centered around 0 V vs Ag/AgCl respectively. CV was performed in 0.5 M Na₂SO₄ aqueous electrolyte with platinum wire counter and Ag/AgCl reference electrodes over a potential window of -0.3 to 0.3 V.

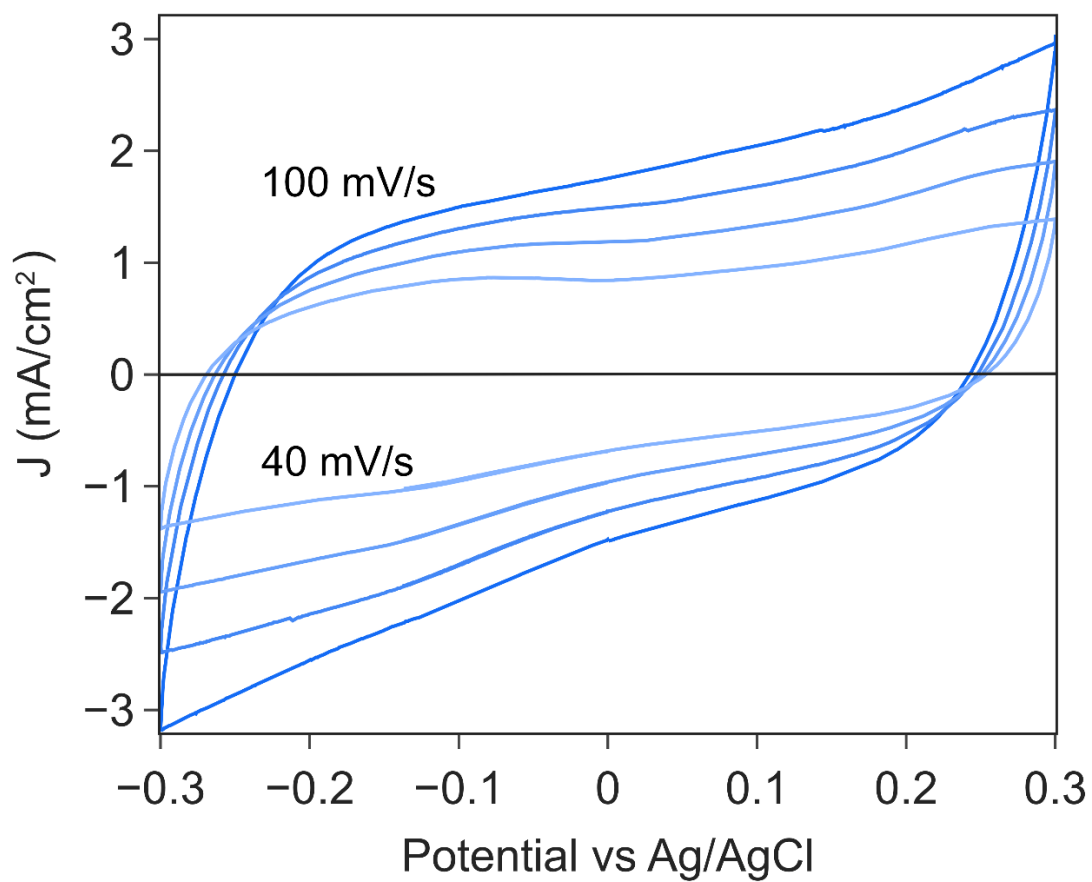


Figure S4. CV of 1T-MoS₂ | Ni | Kapton taken in 0.5 M Na₂SO₄ aqueous electrolyte with platinum wire counter and Ag/AgCl reference electrodes at scan rates of 40, 60, 80, and 100 mV/s.

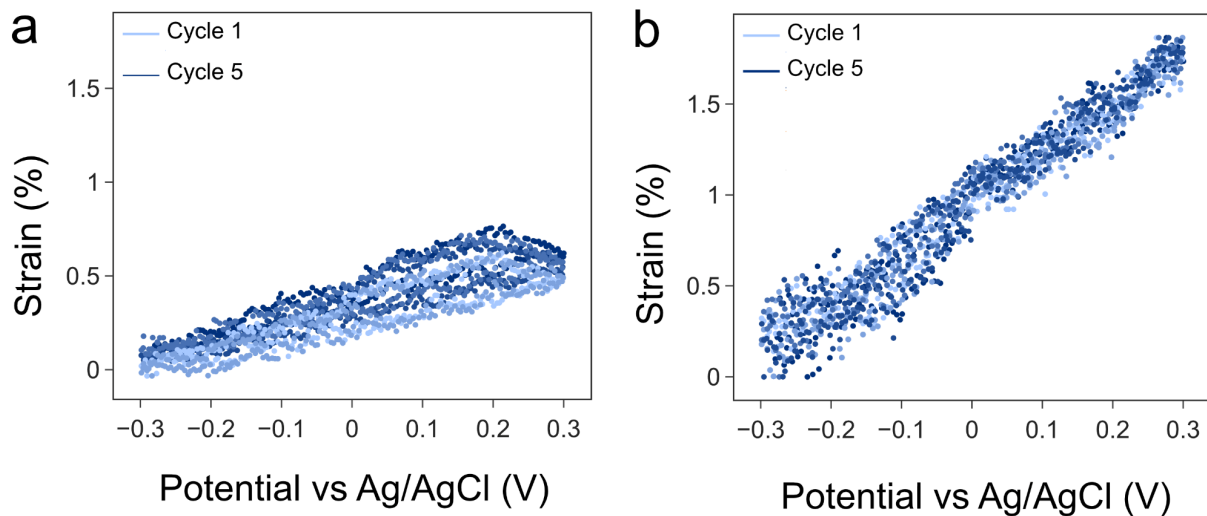


Figure S5. a) Strain % versus potential of 1T-MoS₂ | Ni | Kapton electrode for five cycles. Rearrangement or creep of active layer results in shift in strain % on the Ni substrate but the shape remains consistent. b) Strain % versus potential of 1T-MoS₂ | Au | Kapton electrode for five cycles.

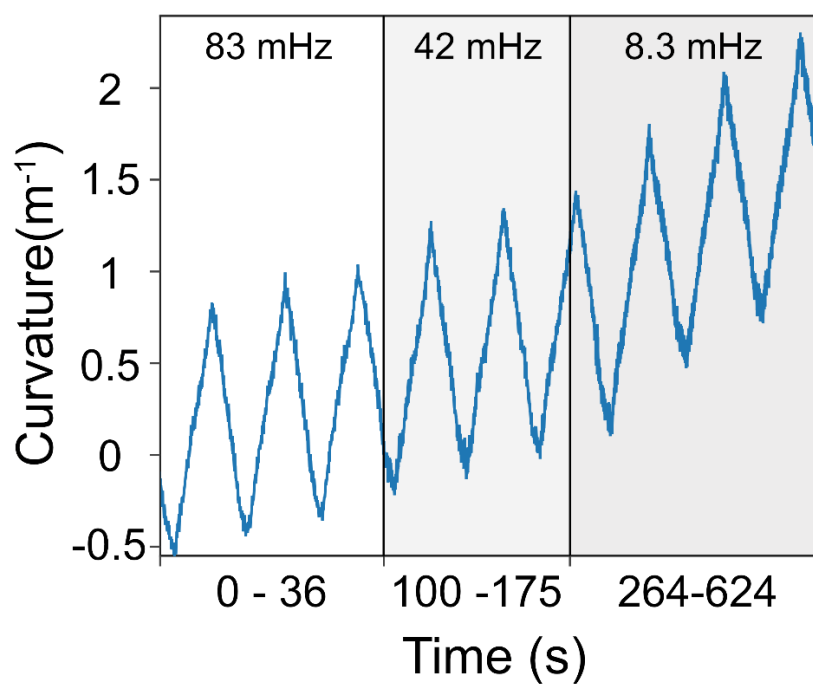


Figure S6. Scan rate dependence of 1T-MoS₂ | Ni | Kapton electrode at scan rates of 100, 50, and 10 mV/s. CV was performed in 0.5 M Na₂SO₄ aqueous electrolyte with platinum wire counter and Ag/AgCl reference over a potential window of -0.3 to 0.3 V. Maximum change in curvature is consistent within error between all three scan rates.

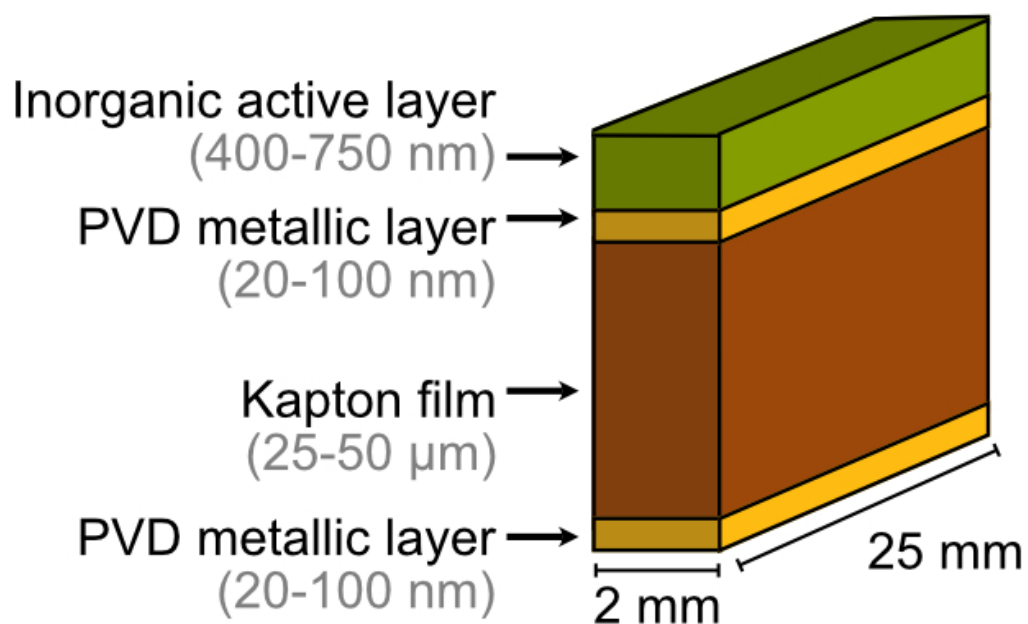


Figure S7. Schematic of $\text{V}_2\text{O}_5 \cdot 0.5 \text{H}_2\text{O} \mid \text{Au} \mid \text{Kapton}$ electrode with double sided metal coatings to prevent issues with swelling of Kapton in organic electrolytes. Electrodes were fabricated by methods described in main text.

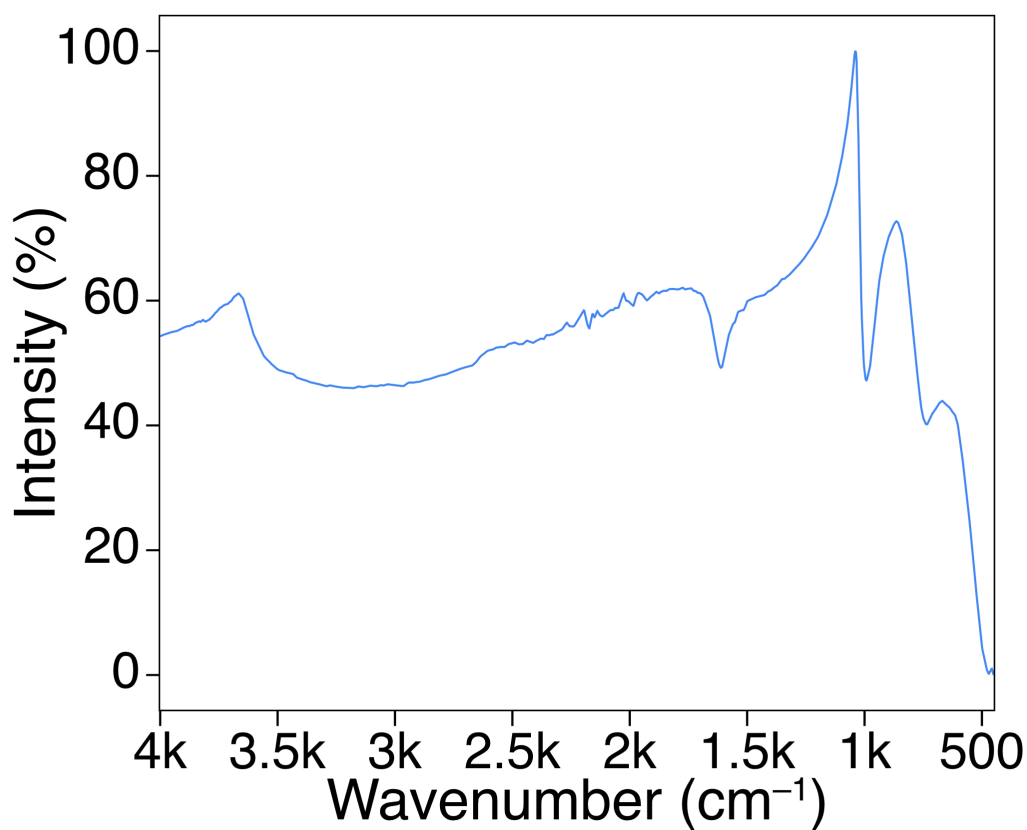


Figure S8. Infrared spectrum of $\text{V}_2\text{O}_5 \cdot 0.5 \text{H}_2\text{O}$ bulk material. Broad hump at 3000 cm^{-1} and peak at 1600 cm^{-1} are due to stretching and bending vibrations of OH groups, peak at 992 cm^{-1} is vanadyl stretching vibration ($\text{V}=\text{O}$), and peaks at 738 and 472 cm^{-1} are due to bridging V-O-V and V-O stretching vibrations respectively.

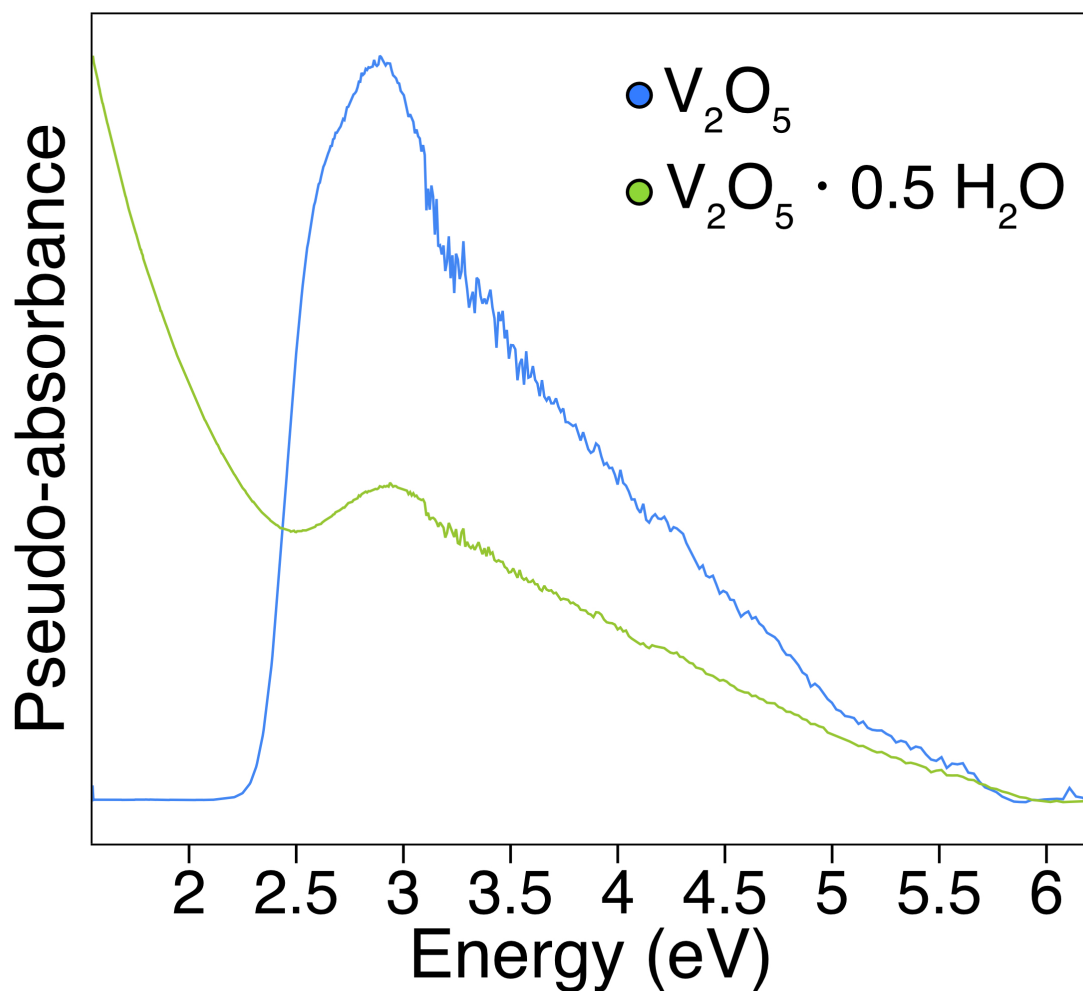


Figure S9. Ultraviolet-visible absorption spectrum (UV-vis) of synthesized $V_2O_5 \cdot 0.5 H_2O$ bulk material and V_2O_5 starting material diffuse reflectance data was converted to pseudo absorbance spectra using Kubelka-Munk transformation. V_2O_5 is initially a bright orange color but during synthesis of hydrate becomes dark green/black color as reflected by increased absorbance in low energy region.

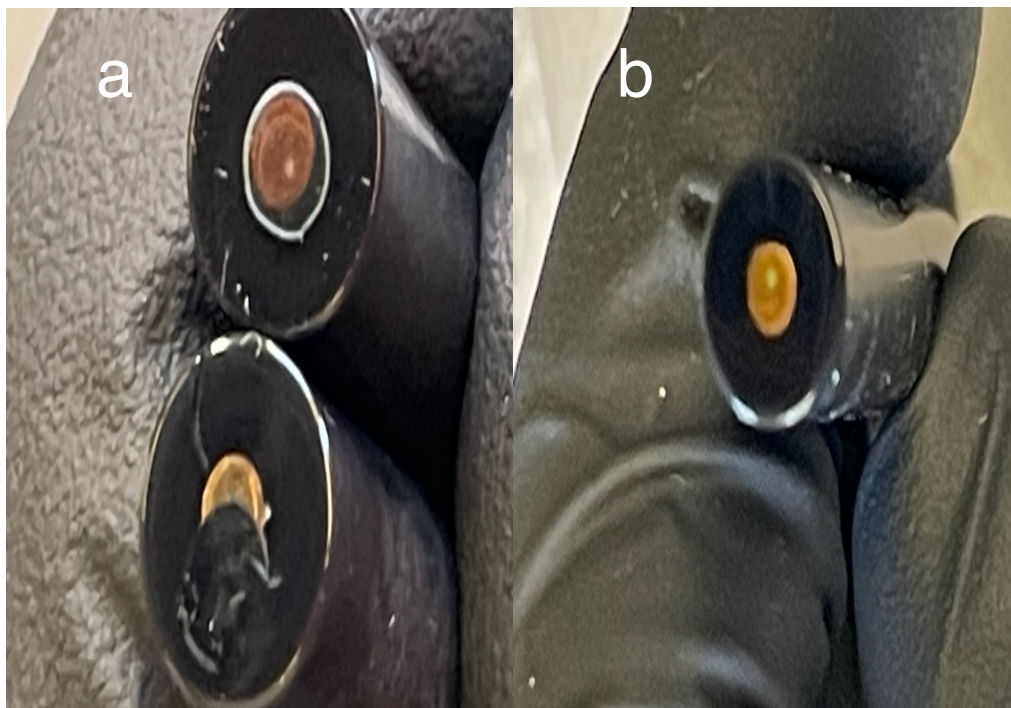


Figure S10. Measurements taken in 0.5 M NaClO₄ propylene carbonate electrolyte with platinum wire counter and Ag/Ag⁺ reference electrodes at scan rate of 0.1 mV/s. (a) Images of V₂O₅ · 0.5 H₂O | Au disc electrodes, top electrode is as prepared by drop casting V₂O₅ · 0.5 H₂O onto Au disc electrodes and drying. After applying at 0 V vs Ag/Ag⁺ for 30 minutes, the V₂O₅ · 0.5 H₂O film became a dark black seen in the bottom electrode. (b) Image of V₂O₅ · 0.5 H₂O | Au disc electrode after holding at 1.3 V vs Ag/Ag⁺ for 30 minutes after having cycled the electrode within a potential window of 0 V to 1.3 V 10 times. Return of orange color of V₂O₅ · 0.5 H₂O film is due to oxidation of V⁴⁺ to V⁵⁺ showing reversibility of electrochemical reaction.

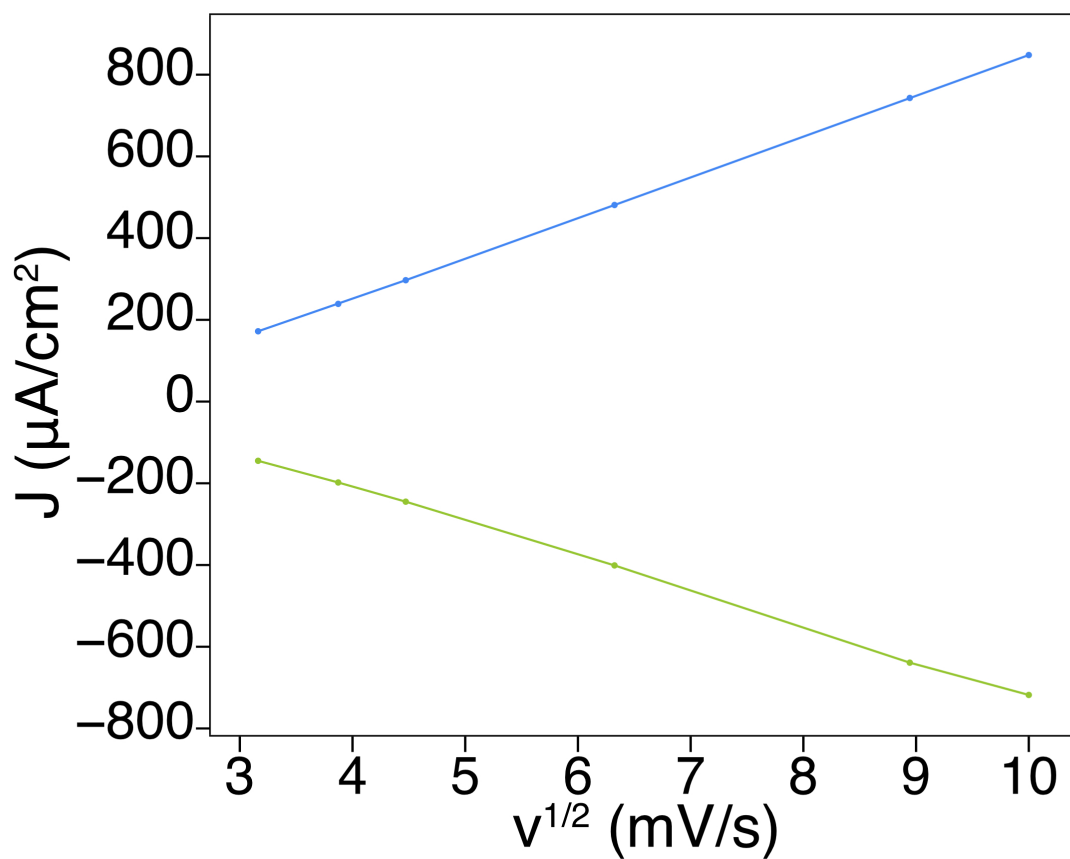


Figure S11. Plots of peak current density J ($\mu\text{A}/\text{cm}^2$) versus square root of the scan rate in a $\text{V}_2\text{O}_5 \cdot 0.5 \text{H}_2\text{O} \mid \text{Au} \mid \text{Kapton}$ electrode taken in 0.5 M NaClO_4 propylene carbonate electrolyte with platinum wire counter and Ag/AgNO_3 reference electrodes at scan rates of 10, 15, 20, 40, 80, and 100 mV/s. Linearity of the plot indicates a reversible diffusion limited process.

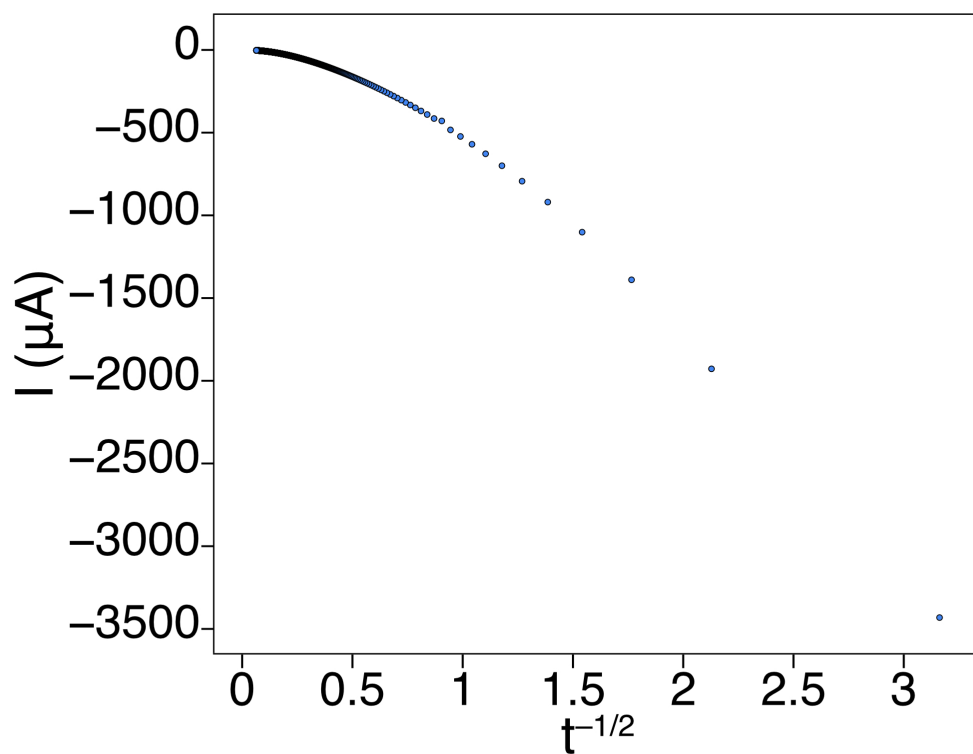


Figure S12. Plot of current (μA) versus inverse square root of time ($\text{s}^{-1/2}$) in a $\text{V}_2\text{O}_5 \cdot 0.5 \text{H}_2\text{O} \mid \text{Au} \mid \text{Kapton}$ electrode taken in 0.5 M NaClO_4 propylene carbonate electrolyte with platinum wire counter and Ag/AgNO_3 reference electrodes at potential limits of -0.8 V and 1.0 V and held for 4 minutes. Linearity of the plot indicates a reversible Cottrell diffusion limited process.

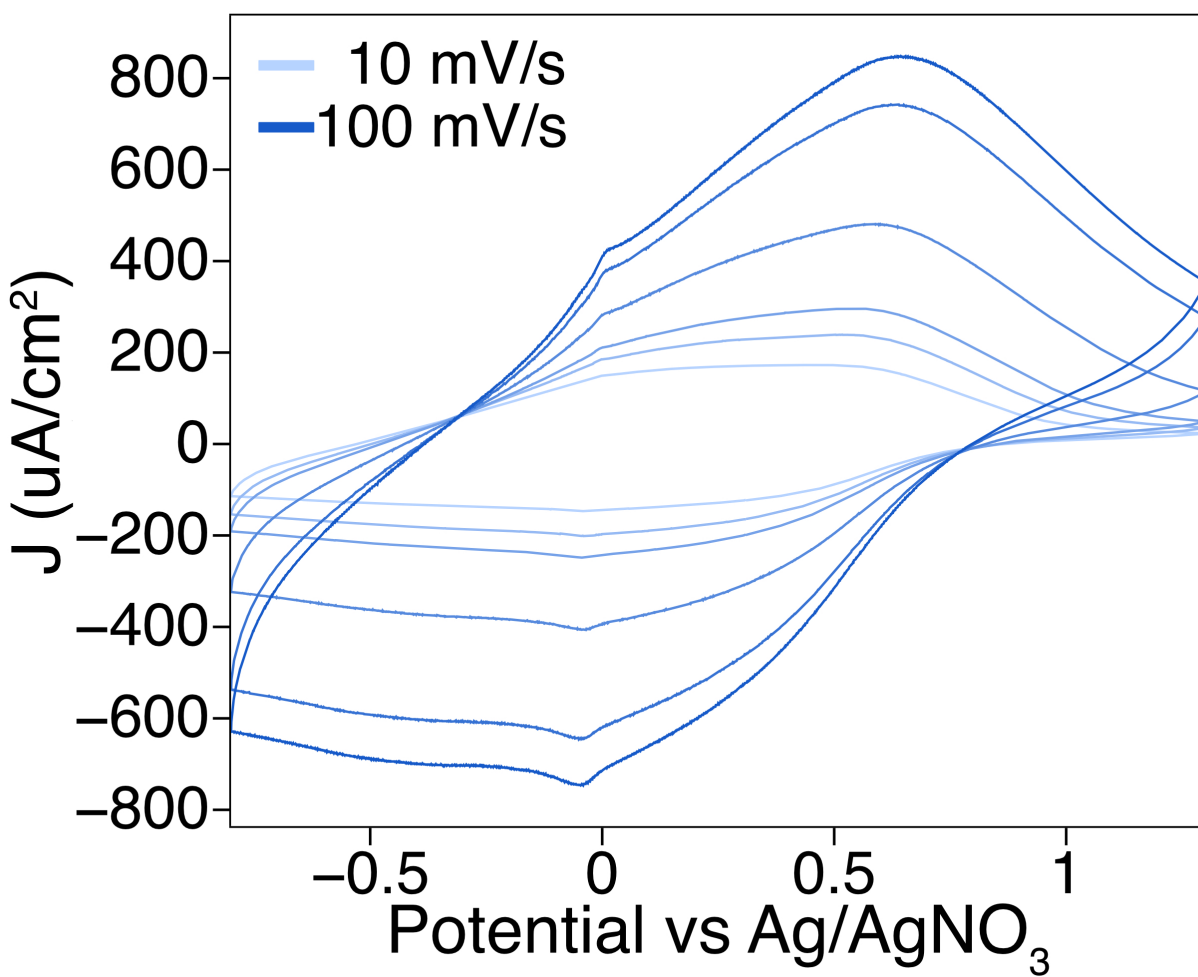


Figure S13. CV of $\text{V}_2\text{O}_5 \cdot 0.5 \text{H}_2\text{O} | \text{Au} | \text{Kapton}$ taken in 0.5 M NaClO_4 propylene carbonate electrolyte with platinum wire counter and Ag/AgNO_3 reference electrodes at scan rates of 10, 15, 20, 40, 80, and 100 mV/s.

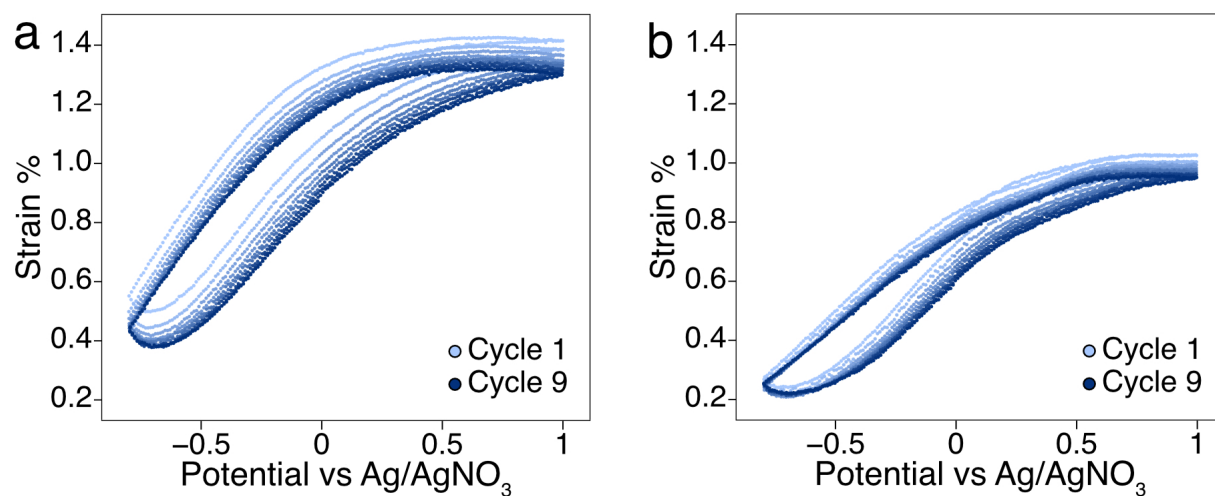


Figure S14. a) Strain % versus potential of V₂O₅ · 0.5 H₂O | Ni | Kapton electrode for nine cycles. During initial cycles rearrangement or creep of active layer results in shift in strain % achieved but stabilizes with further cycling. b) Strain % versus potential of V₂O₅ · 0.5 H₂O | Au | Kapton electrode for nine cycles.

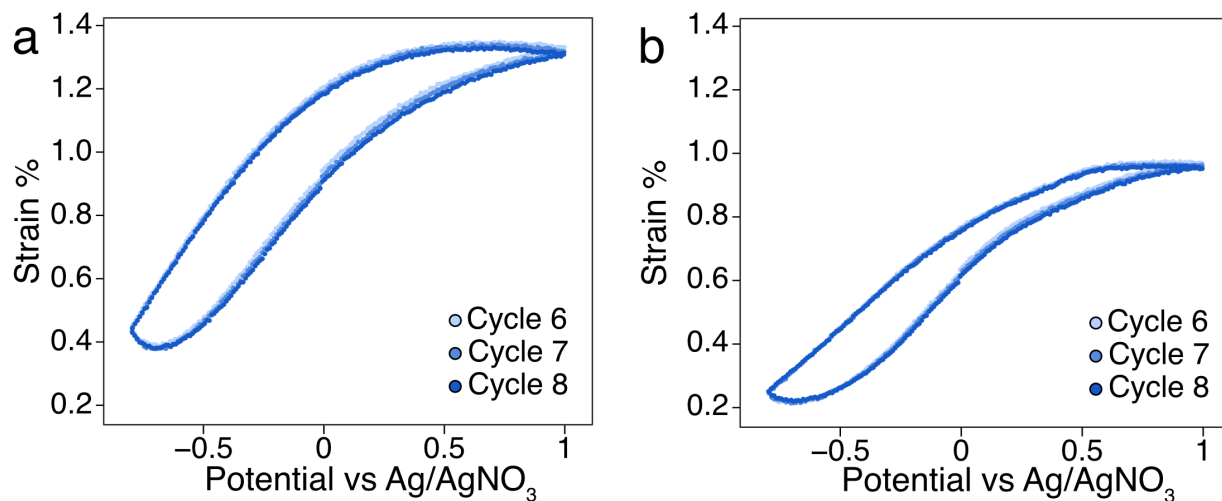


Figure S15. a) Strain % versus potential of V₂O₅ · 0.5 H₂O | Ni | Kapton electrode for three cycles after creep/rearrangement of active layer. b) Strain % versus potential of V₂O₅ · 0.5 H₂O | Au | Kapton electrode for three cycles after creep/rearrangement of active layer.

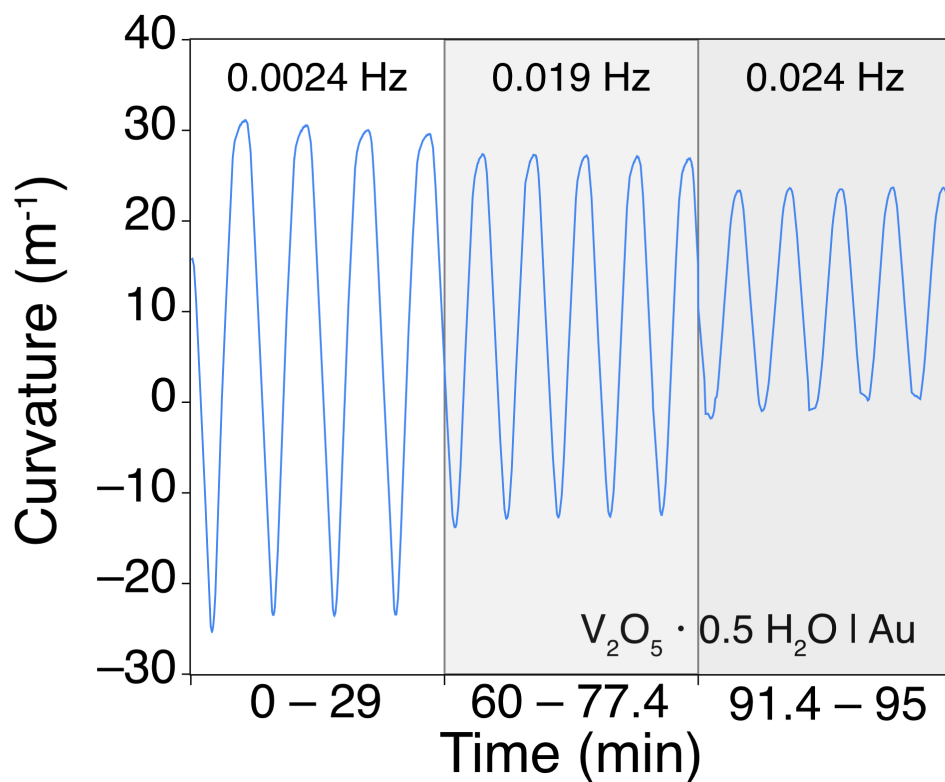


Figure S16. Scan rate dependence of $\text{V}_2\text{O}_5 \cdot 0.5 \text{H}_2\text{O} | \text{Au} | \text{Kapton}$ electrode at scan rates of 10, 40, and 100 mV/s taken in 0.5 M NaClO_4 propylene carbonate electrolyte with platinum wire counter and Ag/AgNO_3 reference electrodes.

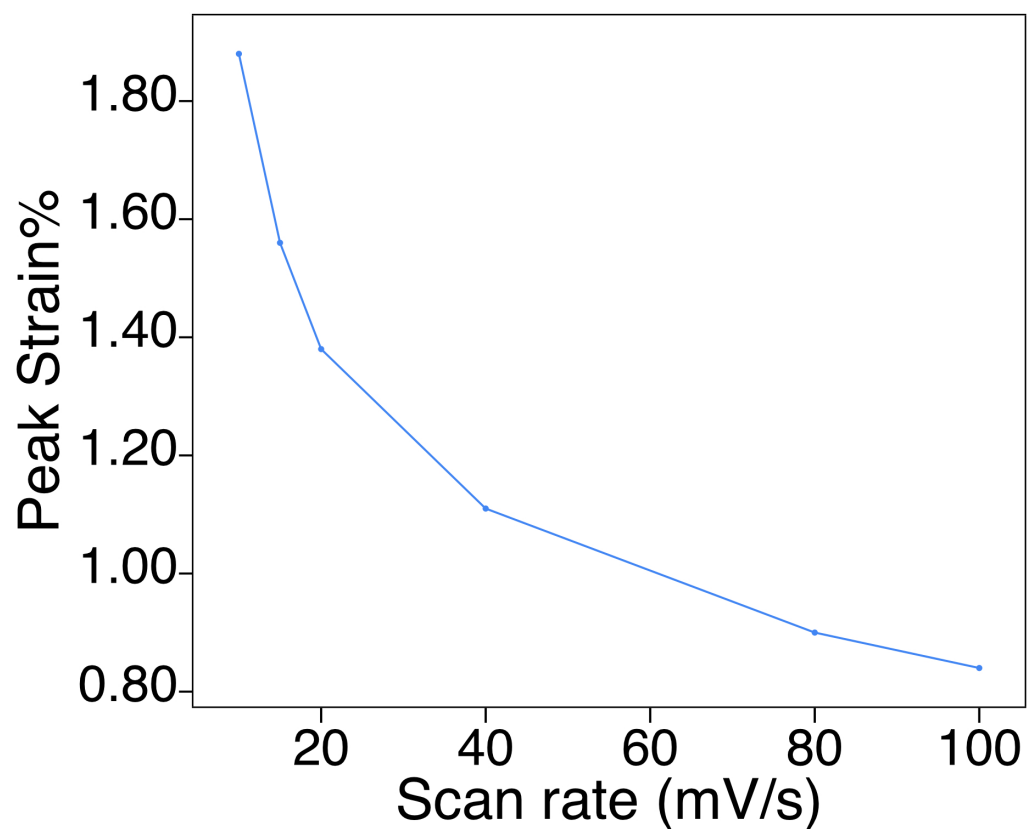


Figure S17. Peak Strain% values calculated during actuation at various potential scan rates in a $\text{V}_2\text{O}_5 \cdot 0.5 \text{H}_2\text{O} \mid \text{Au} \mid \text{Kapton}$ actuator taken in 0.5 M NaClO_4 propylene carbonate electrolyte with platinum wire counter and Ag/AgNO_3 reference electrodes at scan rates of 10, 15, 20, 40, 80, and 100 mV/s.

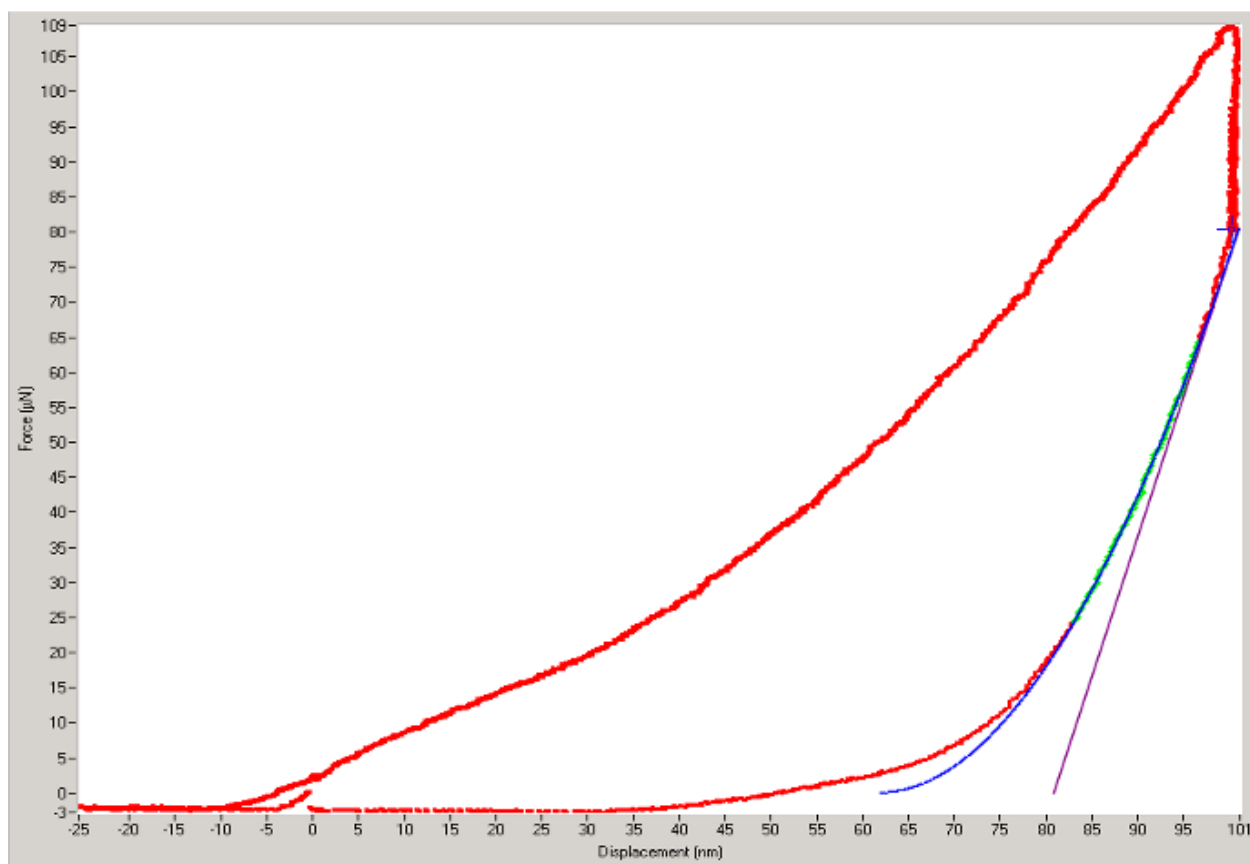


Figure S18. Nanoindentation of deposited $\text{V}_2\text{O}_5 \cdot 0.5 \text{H}_2\text{O}$. Indent depth was kept below $\sim 10\%$ of the active layer thickness to avoid influence from the substrate. Based on the displacement response to the applied force an out of plane Young's modulus of 6.21 GPa and was converted to the in-plane Young's modulus using Acerce's method and the Poisson ratio of V_2O_5 (0.24) which was found as 1.46 GPa.⁶⁷

Table S1. Summary of actuator changes in curvature observed and strains, stress, and moduli calculated based on the known crystallographic strain for $\text{Na}_x\text{V}_2\text{O}_5 \cdot 0.5 \text{H}_2\text{O} \mid \text{M} \mid \text{Kapton}$ electrodes where M is metal layer identity.

Measurement	Curvature	Strain %	Stress (Mpa)	Modulus	Samples
Au-CV	18(3)	1.84(0.10)	16(2)	0.9(1)	6
Au-CA	20(3)	2.15(0.10)	18(3)	0.8(1)	6
Ni-CV	16(1)	2.24(0.12)	11.7(6)	0.56(2)	7
Ni-CA	22(2)	2.47(0.10)	17(1)	0.68(3)	7

Table S2. Stresses due to actuation calculated for $\text{V}_2\text{O}_5 \cdot 0.5 \text{H}_2\text{O} \mid \text{M} \mid \text{Kapton}$ electrodes using the Stoney model where M is the metal layer identity.

Electrode-measurement	Stoney Stress (MPa)
$\text{V}_2\text{O}_5 \cdot 0.5 \text{H}_2\text{O} \mid \text{Au} \mid \text{Kapton-CV}$	15(2)
$\text{V}_2\text{O}_5 \cdot 0.5 \text{H}_2\text{O} \mid \text{Au} \mid \text{Kapton-CA}$	16(2)
$\text{V}_2\text{O}_5 \cdot 0.5 \text{H}_2\text{O} \mid \text{Ni} \mid \text{Kapton-CV}$	10.8(5)
$\text{V}_2\text{O}_5 \cdot 0.5 \text{H}_2\text{O} \mid \text{Ni} \mid \text{Kapton-CA}$	16(1)

Table S3. Stresses due to actuation calculated for $1\text{T-MoS}_2 \mid \text{M} \mid \text{Kapton}$ electrodes using the Stoney model.

Electrode-measurement	Stoney Stress (MPa)
$1\text{T-MoS}_2 \mid \text{Au} \mid \text{Kapton-CV}$	17(2)
$1\text{T-MoS}_2 \mid \text{Au} \mid \text{Kapton-CA}$	15.3(0.8)
$1\text{T-MoS}_2 \mid \text{Ni} \mid \text{Kapton-CV}$	5.3(0.5)
$1\text{T-MoS}_2 \mid \text{Ni} \mid \text{Kapton-CA}$	4.5(0.4)

Table S4. Summary of reported V₂O₅ based actuators Strain %, active layer modulus, generated Stress, and fabrication method where NW is nanowires, SWCNT is single walled carbon nanotubes, and CNTF is carbon nanotube fiber.

Actuator	Strain %	Modulus (Gpa)	Stress (Mpa)	Fabrication	Reference
V ₂ O ₅ NWs	0.21	4.8	5.9	Entangled nanowires in cellulose filter by vacuum filtration	12
V ₂ O ₅ NW/SWCNT	0.18	NR	1.54E-03	Entangled V ₂ O ₅ and SWCNT by vacuum filtration	78
V ₂ O ₅ NW/CNTF	NR	15.4	NR	Wet twisting V ₂ O ₅ NW and CNTF	24
V ₂ O ₅ · 0.5 H ₂ O Au	1.24(0.20)	1.46	18(3)	Wet cast thin film	This work
V ₂ O ₅ · 0.5 H ₂ O Ni	1.17(0.08)	1.46	17(1)	Wet cast thin film	This work

Table S5. Summary of reported MoS₂ based actuators Strain %, active layer modulus, generated Stress, and fabrication method where pMoS₂-nSNrGO is oxide-doped p-type MoS₂ and sulfur-nitrogen-doped n-type graphene, PDMS is polydimethylsiloxane, and PVDF is polyvinylidene difluoride.

Actuator	Strain %	Modulus (Gpa)	Stress (Mpa)	Fabrication	Reference
Polymer nanocomposite	2-5	NR	0.03	2 wt. % ultrafine 2H-MoS ₂ powder in PDMS	79
MoS ₂ -carbon nanotube-polymer	0.76	0.571-0.771	NR	Bulk 2H-MoS ₂ powder mixed with PVDF and carbon nanotubes and dried into a gel	80
pMoS ₂ -nSNrGO nanohybrid	1.2	0.106	NR	Hydrothermal synthesis of “flower-like” nanohybrid, MoS ₂ nanoparticles atop graphene petals	81
1T-MoS ₂ nanosheets	0.6	2-4	17	Restacked nanosheets from liquid suspension by vacuum filtration over nitrocellulose membrane and subsequent transfer to Au-Kapton substrate	82
1T-MoS ₂ film on PVDF	NR	0.0986	NR	Restacked nanosheets from liquid suspension by vacuum filtration over PVDF membrane	83
MoS ₂ Au	1.29(0.13)	1.50	15(1)	Wet cast thin film	This work
MoS ₂ Ni	0.57(0.05)	1.50	7.8(0.6)	Wet cast thin film	This work

References:

78. Y. Ling, H. Fan, K. Wang, Z. Lu, L. Wang, C. Hou, Q. Zhang, Y. Li, K. Li and H. Wang, *Small*, 2022, 18, 2107778.
79. X. Fan, F. Khosravi, V. Rahneshein, M. Shanmugam, M. Loeian, J. Jasinski, R. W. Cohn, E. Terentjev, B. Panchapakesan, *Nanotechnology*, 2015, 26, 261001.
80. D. Gendron, G. Bubak, L. Ceseracciu, F. Ricciardella, A. Ansaldo, D. Ricci, *Sens. Actuators. B. Chem.*, 2016, 230, 673-683
81. M. T. Manzoor, V. H. Nguyen, S. Umrao, J. -H. Kim, R. Tabassian, J. -E. Kim, I. -K. Oh, *Adv. Funct. Mater.*, 2019, 29, 1905454.
82. M. Acerce, E. K. Akdogan and M. Chhowalla, *Nature*, 2017, 549, 370–373.
83. H. Li, H. Yang, C. Xu, X. Cheng, J. Yan, K. Cen, Z. Bao, K. Ostrikov, *J. Thermal Sci. Eng. Appl.*, 2022, 14, 125001.