



# **Designing Oxide Heterostructures for Advanced Electronic and Energy applications**

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**Department of Physics**

**Hankuk University of Foreign Studies**

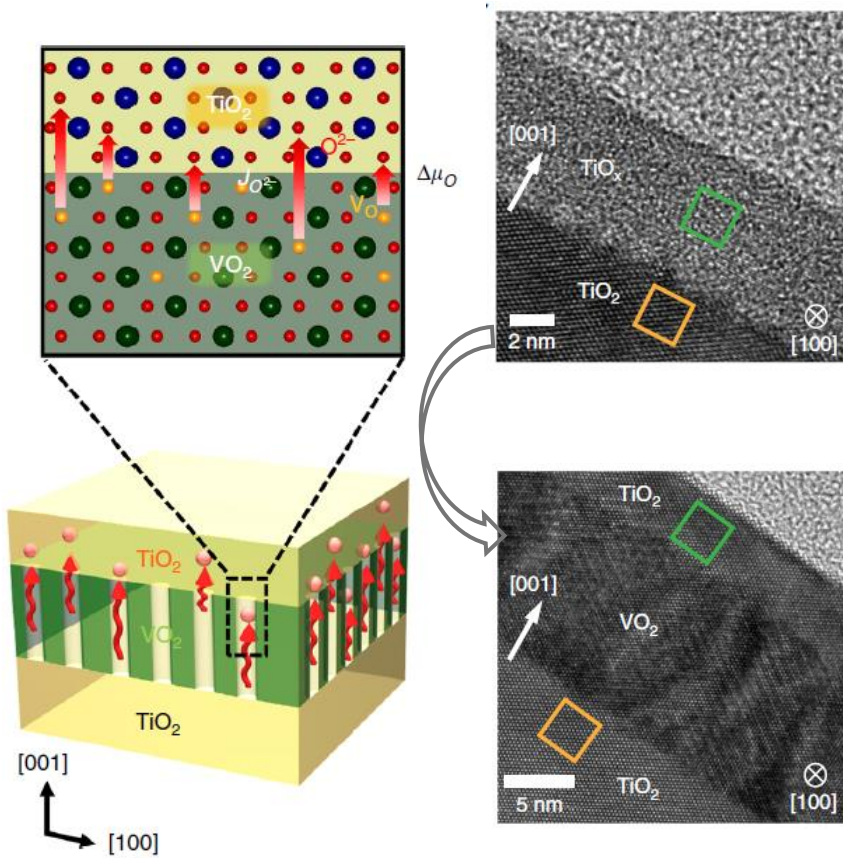
# Contents

- Introduction - Requirement of energy-efficient system
- Topic 1 – Zero-strain metal-insulator transition
- Topic 2 – 2D vacancy formation in oxide homo interfaces
- Summary



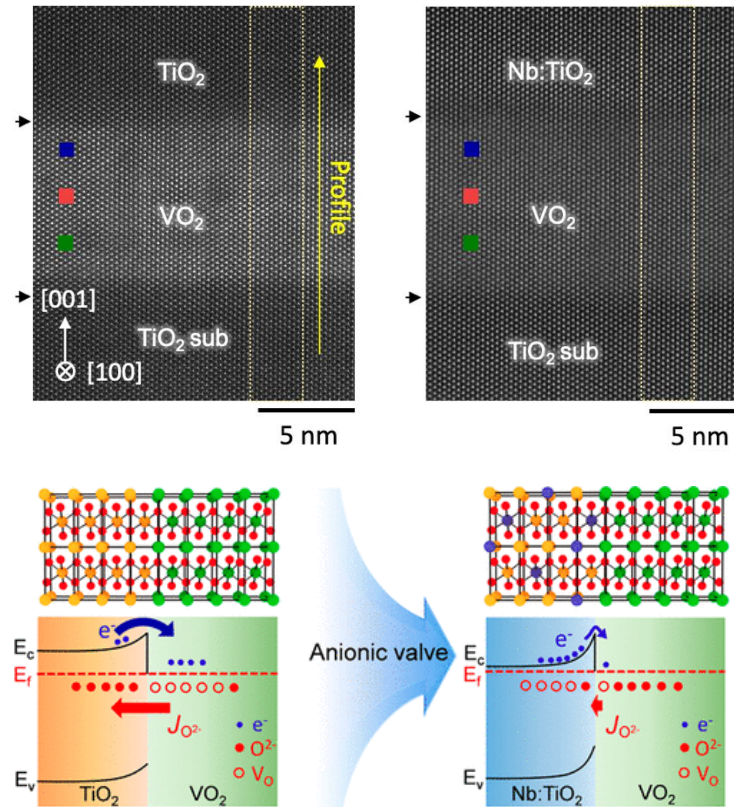
# Previous studies (at POSTECH)

## Low-temperature epitaxy



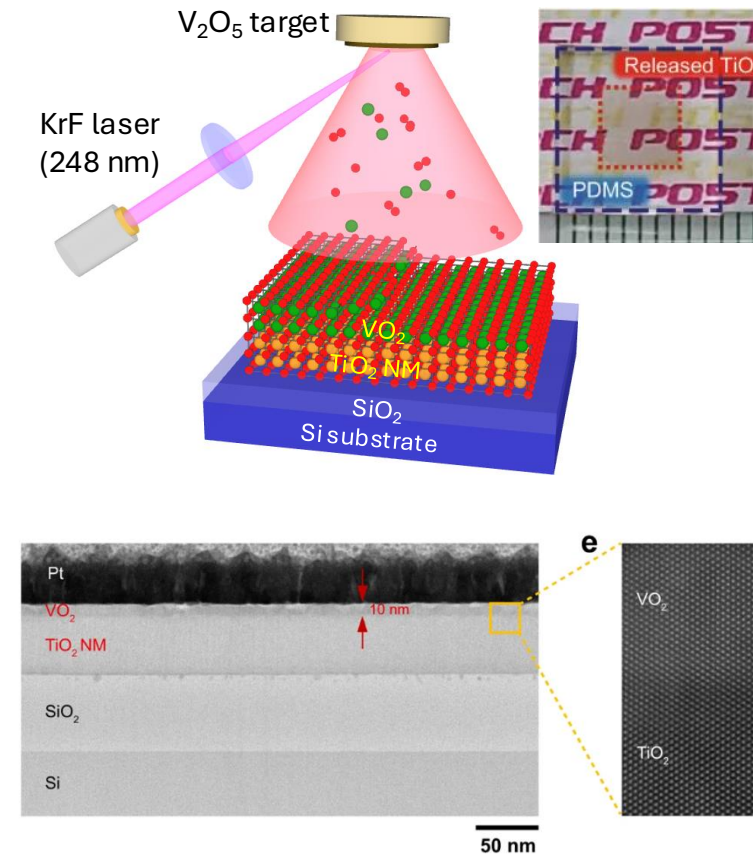
*Nat. Commun.* **11**, 1401 (2020)

## Ionic flow valve



*Nano. Lett.* **22**, 9306-9312 (2022)

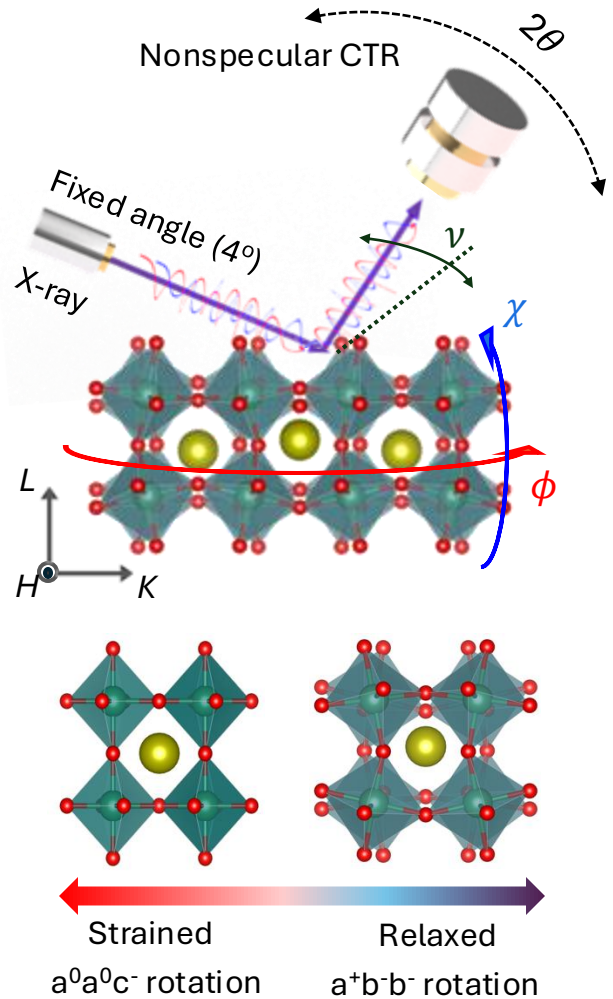
## M3D using freestanding NM



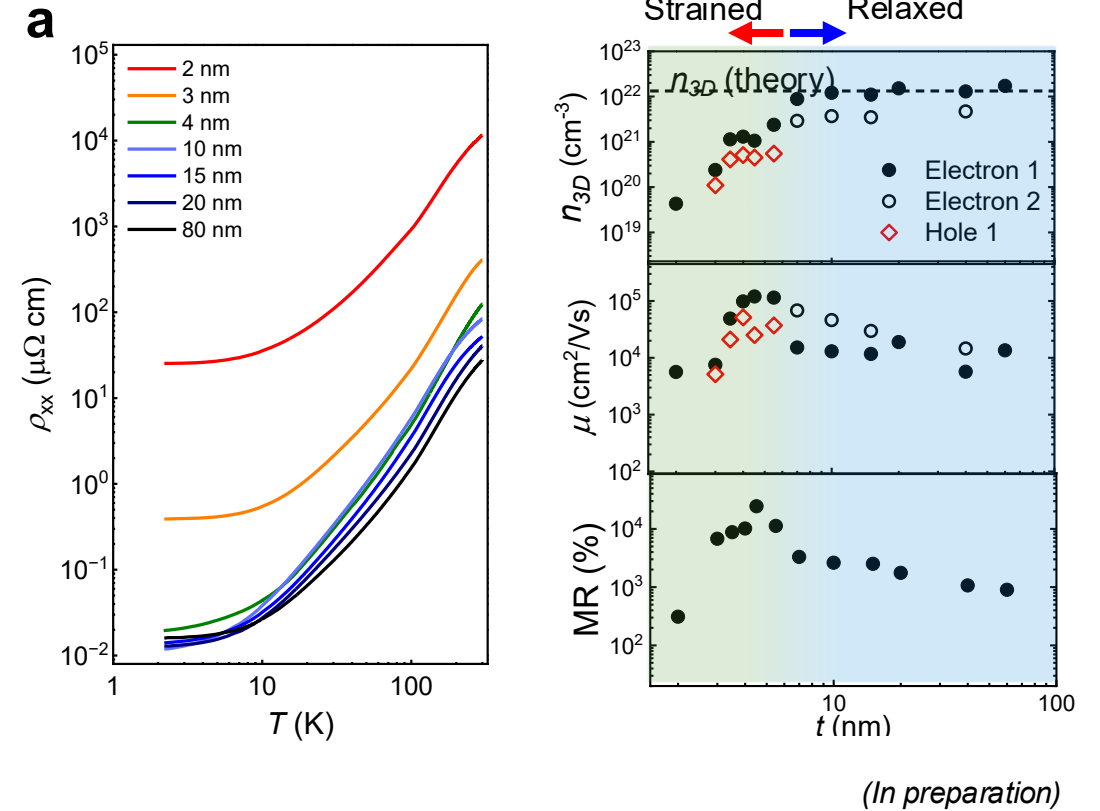
*Nat. Commun.* **12**, 5019 (2021)

# Previous studies (at ORNL)

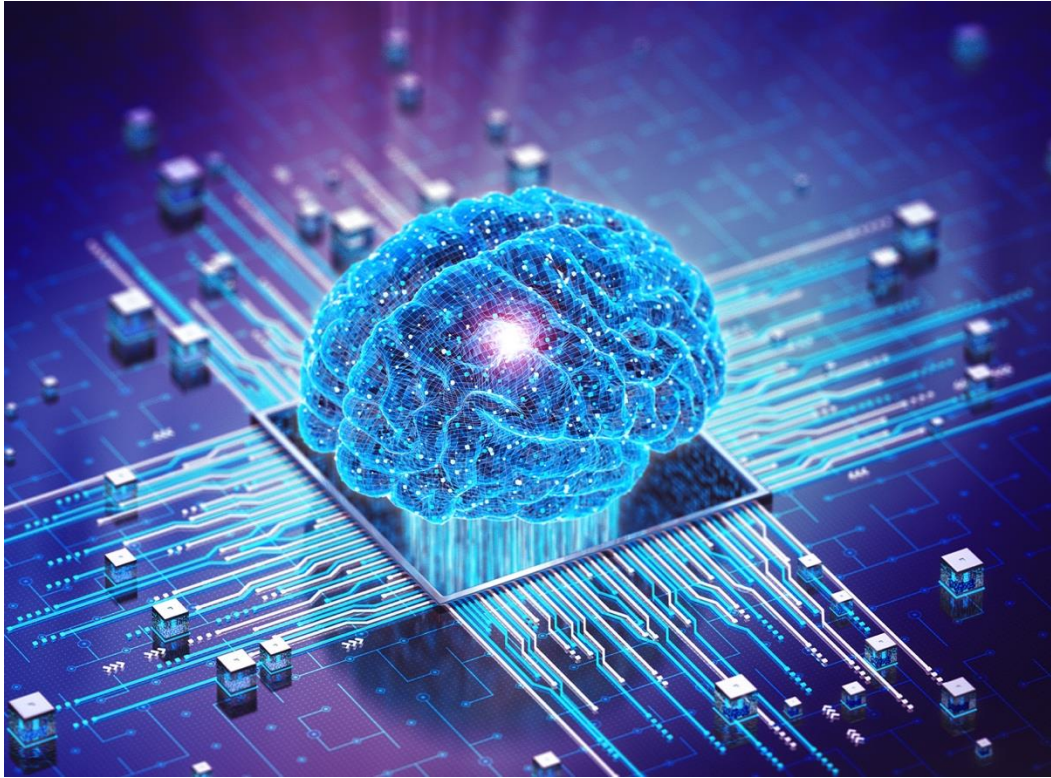
## □ OOR in perovskite QMs



## □ High electron mobility in perovskite QMs



# Development of AI



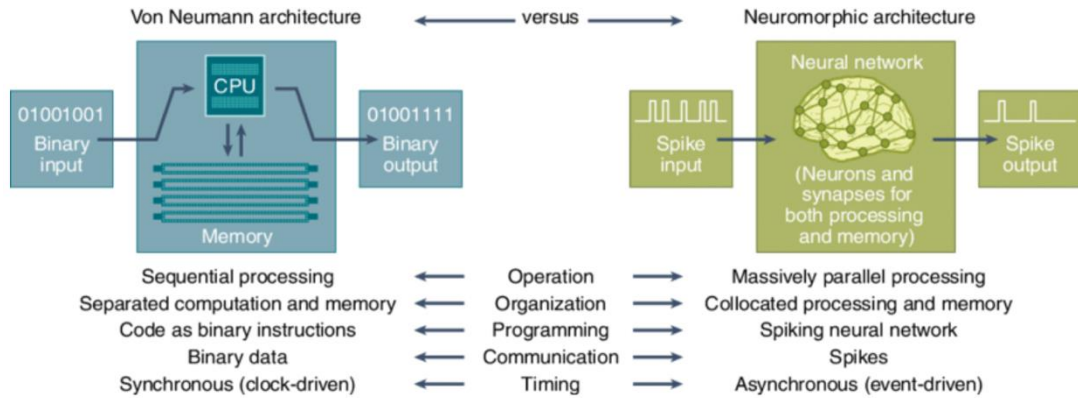
(Image credit: BlackJack3D via Getty Images)



(Image credit: IBM)

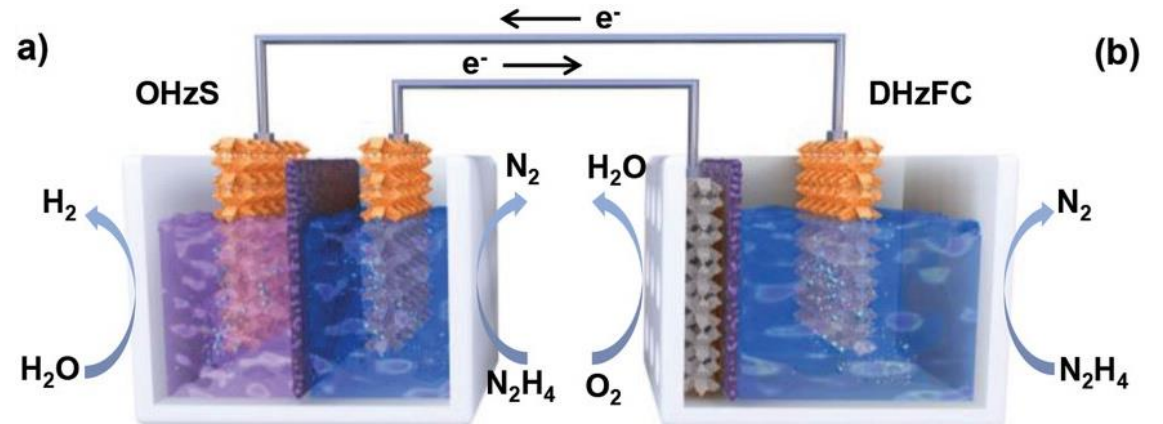
# Pathway for the energy efficient system

## Energy consumption

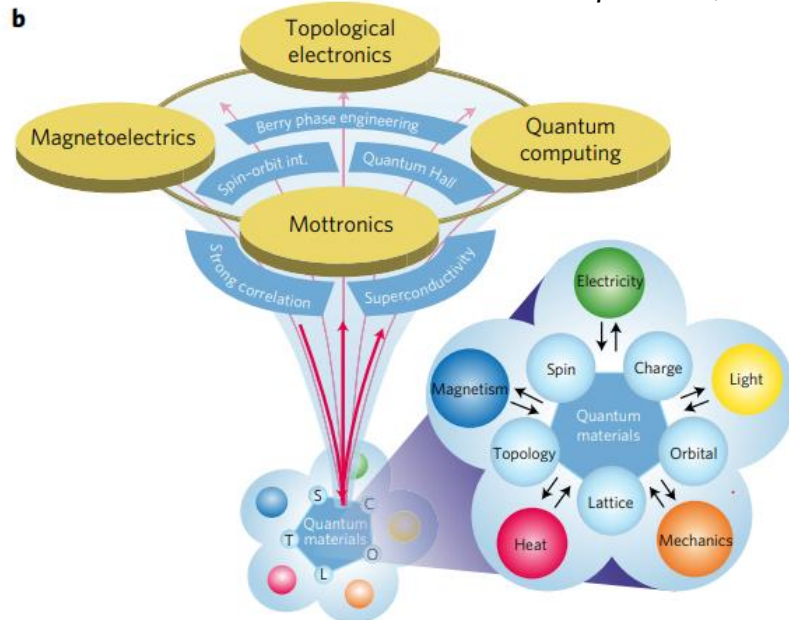


*Nat. Comp. Sci.* **2**, 10-19 (2022)

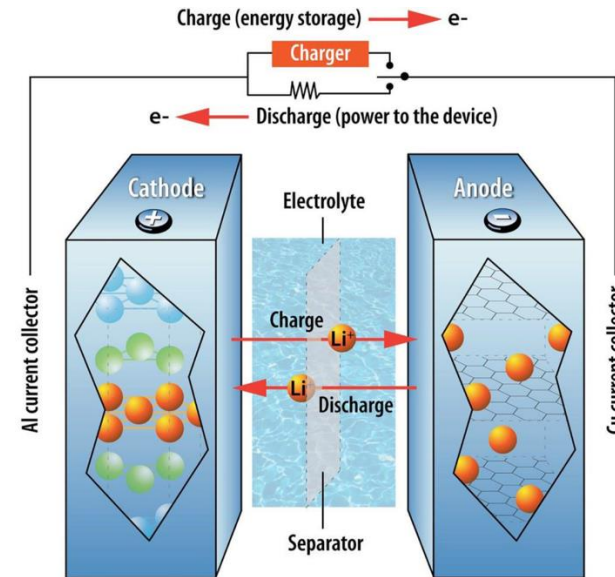
## Energy generation



*Adv. Funct. Mater.* **33**, 2300625 (2023)

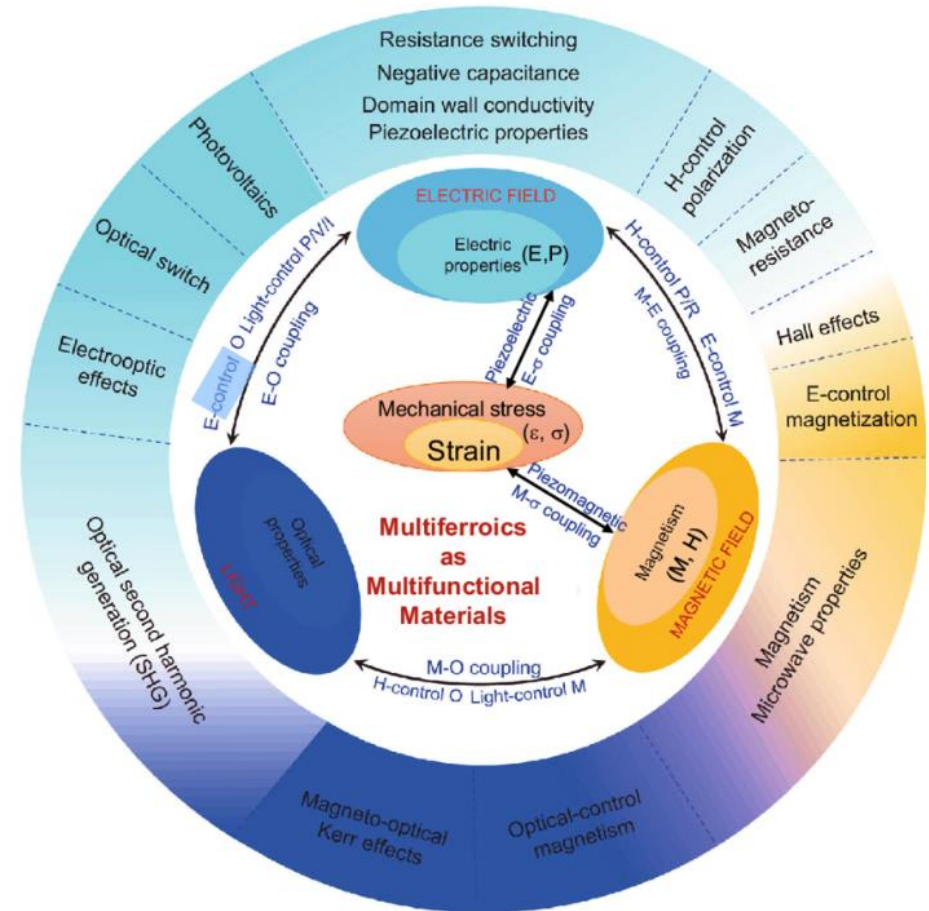
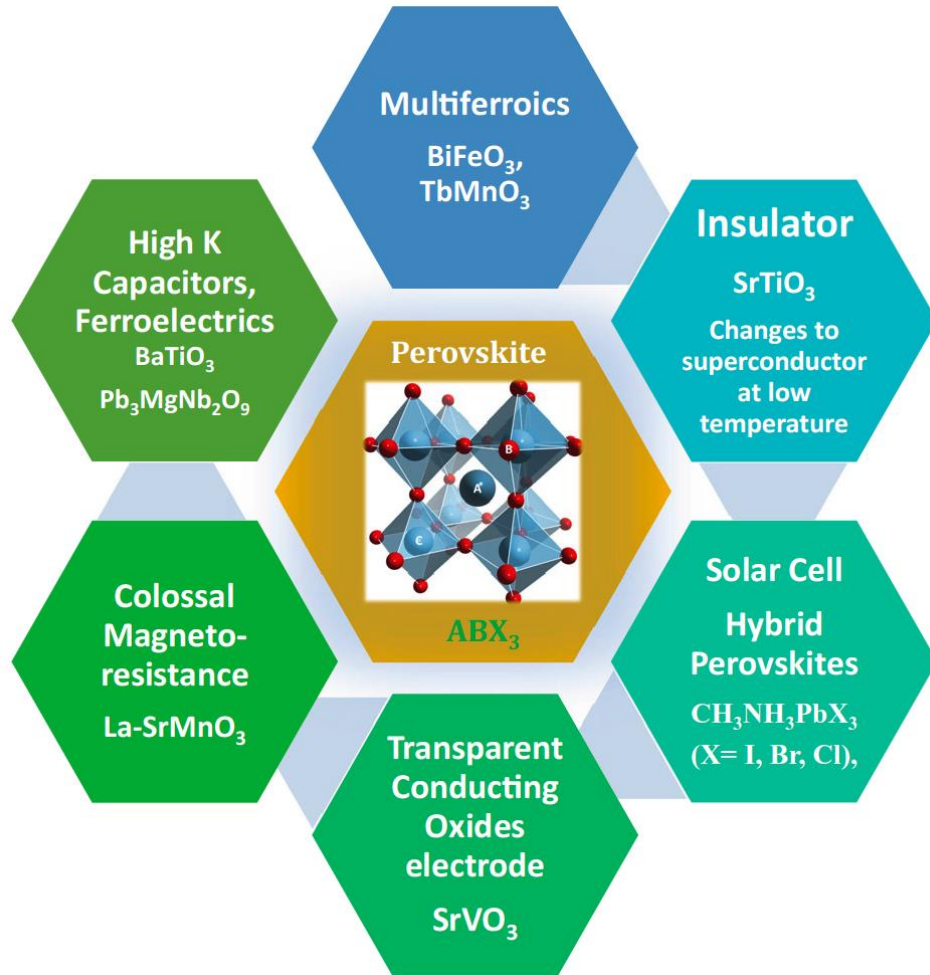


*Nat. Phys.* **13**, 1056-1068(2017)



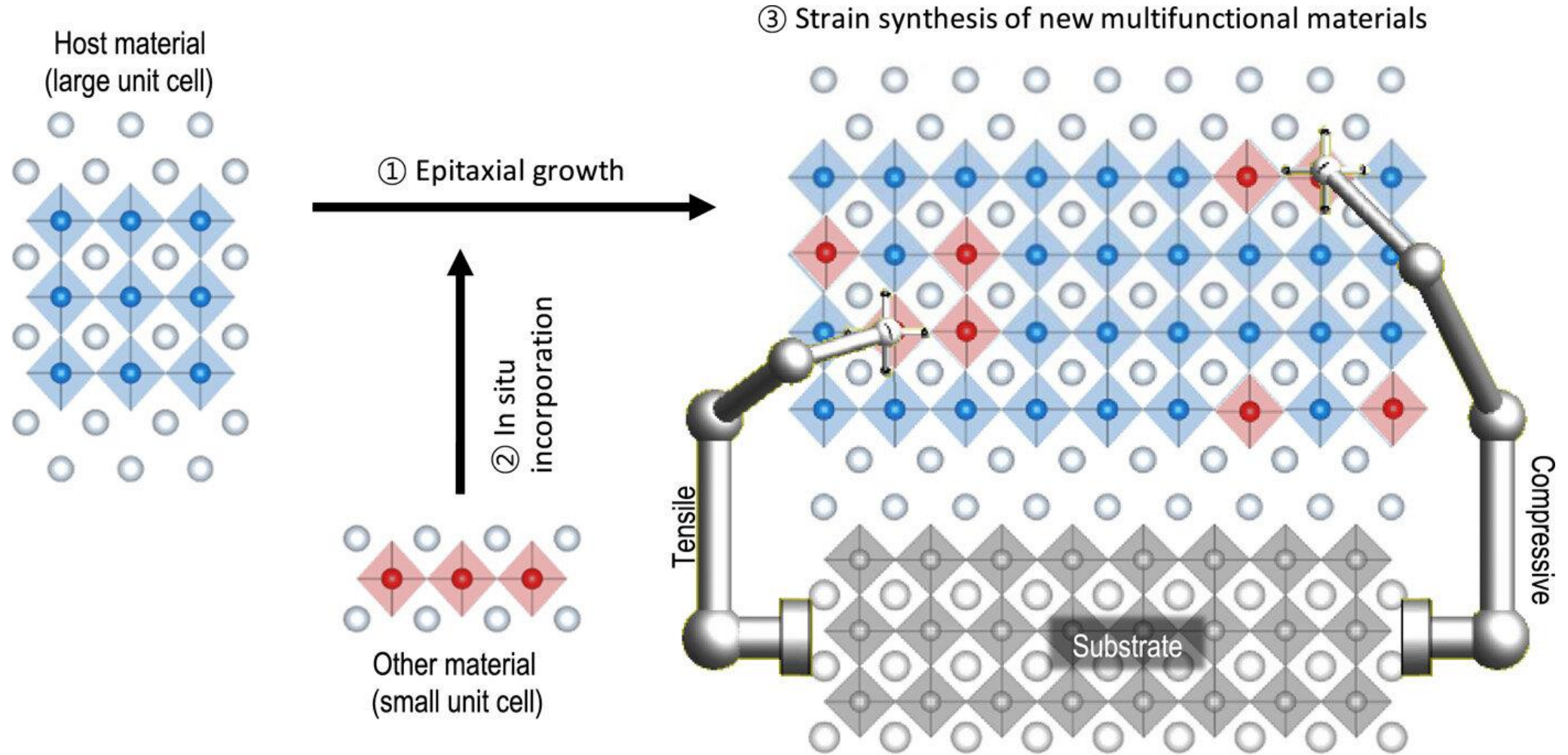
*Appl. Surf. Sci. Adv.* **9** 100233 (2022)

# Opportunities in transition metal oxides



“Structural Perspective on Multifunctional Oxide Materials” Harshit Agarwal (2024)

# Designing of oxide thin films & heterostructures

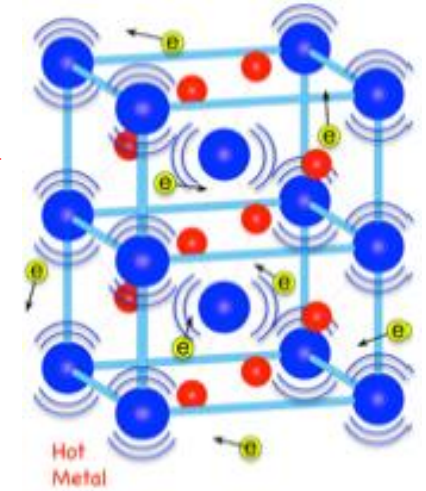
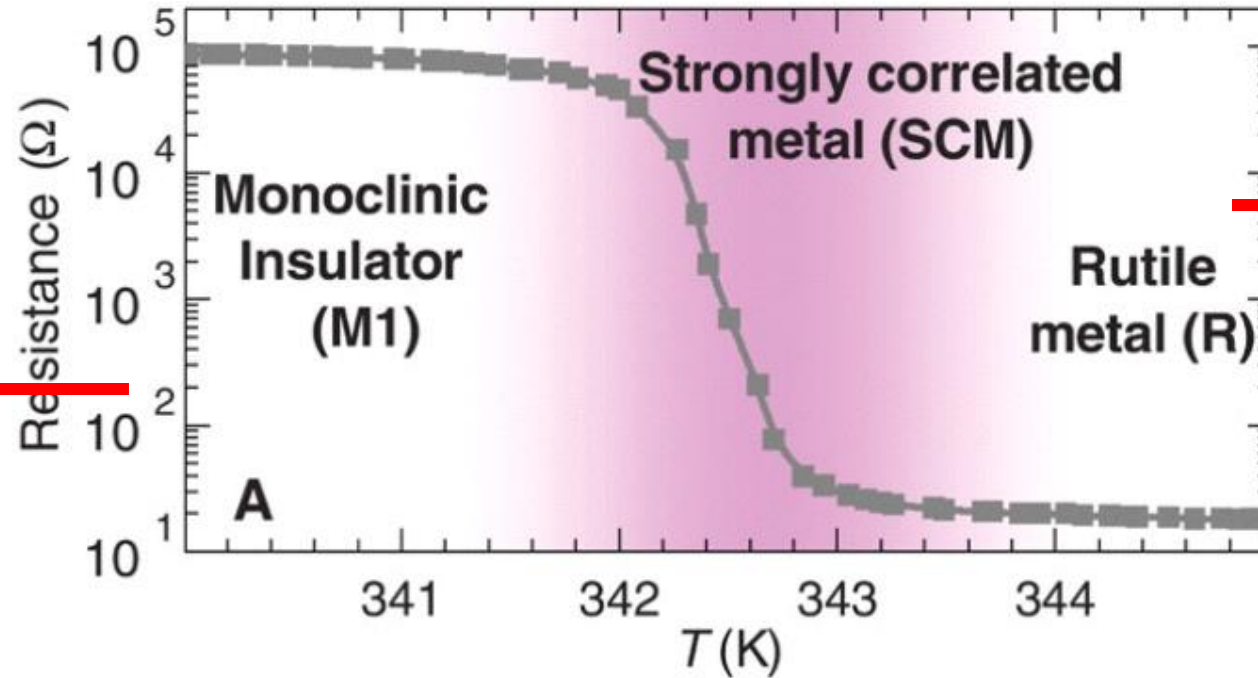
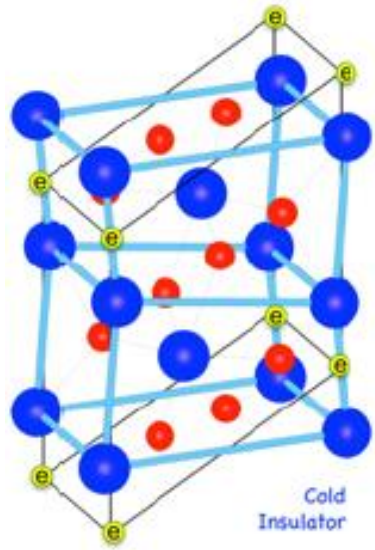


# Contents

- ❑ Topic 1 – Zero-strain metal-insulator transition for ultrafast and energy-efficient threshold switches
- ❑ Topic 2 – 2D vacancy formation in oxide homo interfaces for enhanced PEC activities



# Vanadium dioxide ( $\text{VO}_2$ )



*Science* **318**, 1750 (2007)  
*Phys. Rev. Lett.* **3**, 1 (1959)

VOLUME 3, NUMBER 1

PHYSICAL REVIEW LETTERS

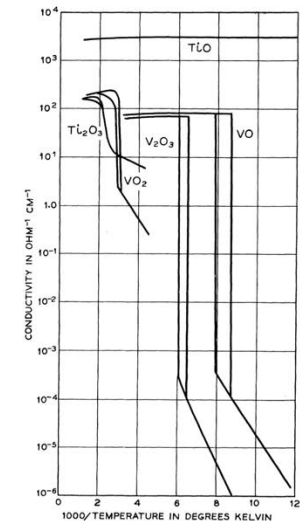
JULY 1, 1959

## OXIDES WHICH SHOW A METAL-TO-INSULATOR TRANSITION AT THE NEEL TEMPERATURE

F. J. Morin

Bell Telephone Laboratories, Murray Hill, New Jersey

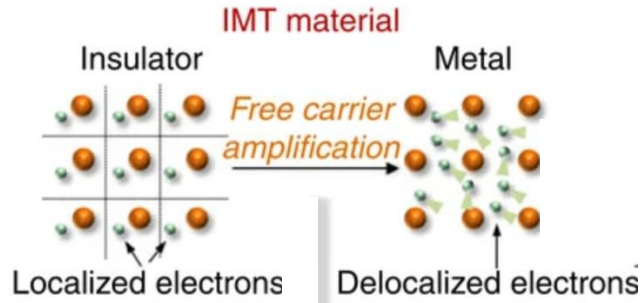
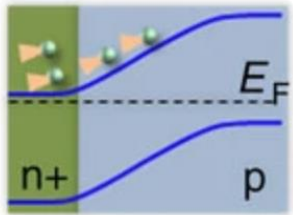
(Received June 5, 1959)



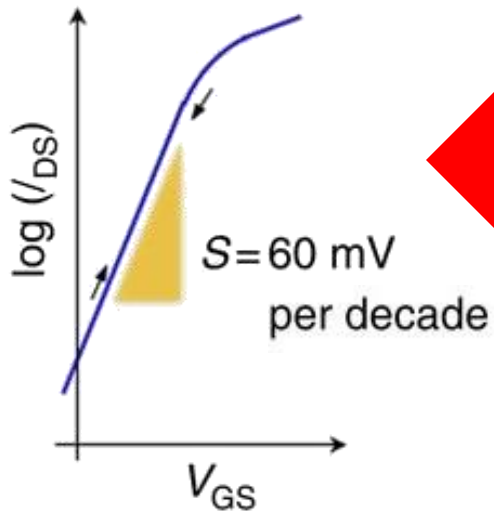
# Possible applications of VO<sub>2</sub>

## Overcoming Boltzmann limit

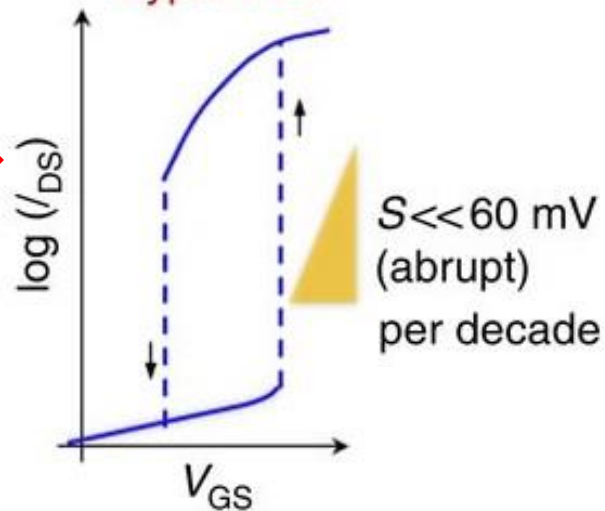
Channel-source  
p-n junction



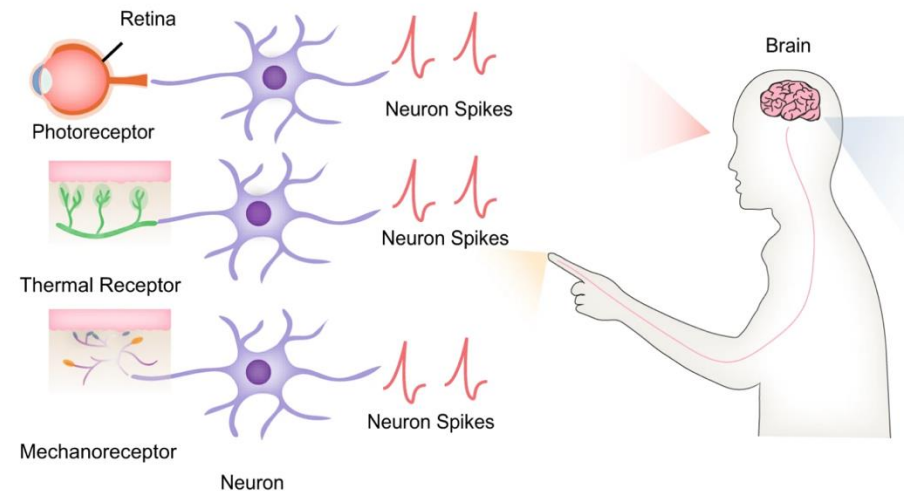
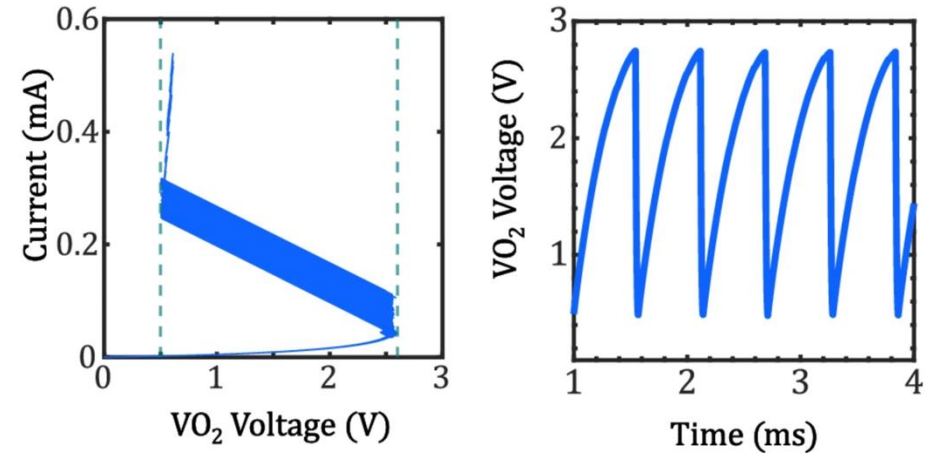
MOSFET



Hyper-FET



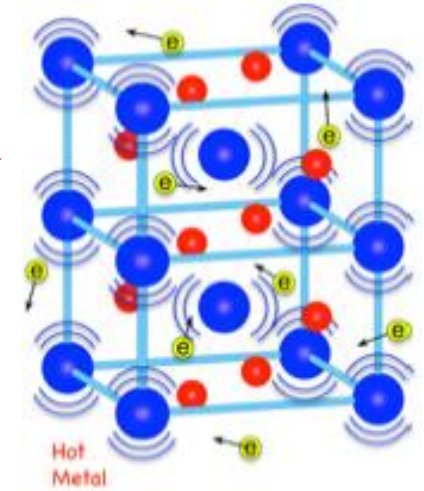
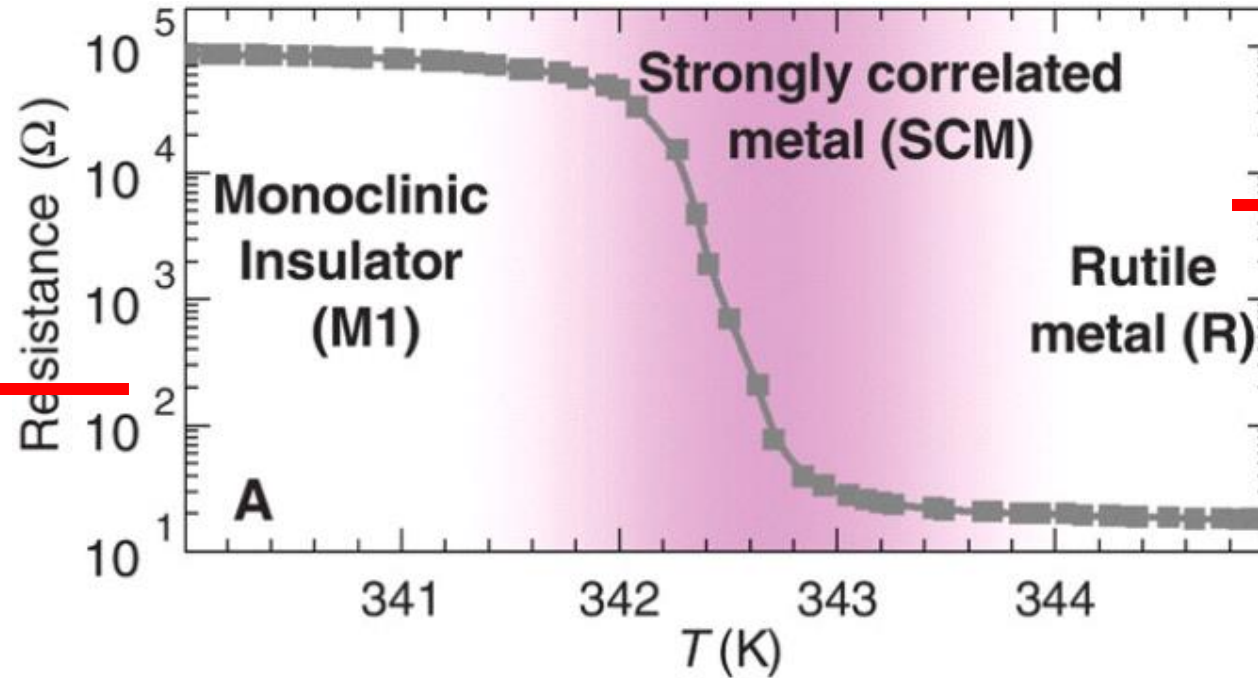
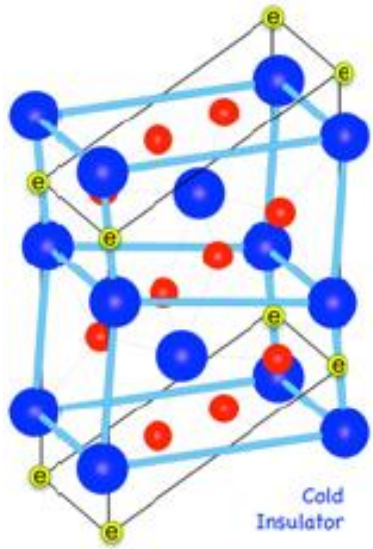
## Neuromorphic applications



*Nat. Commun.* **13**, 3973 (2022)  
*Nat. Commun.* **15**, 3334 (2024)

*Nat. Commun.* **6**, 7812 (2015)

# Origin of the metal-insulator transition



*Science* **318**, 1750 (2007)

*Phys. Rev. Lett.* **3**, 1 (1959)

VOLUME 72, NUMBER 21

PHYSICAL REVIEW LETTERS

23 MAY 1994

## VO<sub>2</sub>: Peierls or Mott-Hubbard? A View from Band Theory

Renata M. Wentzcovitch\*

*Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, United Kingdom*

Werner W. Schulz<sup>†</sup> and Philip B. Allen

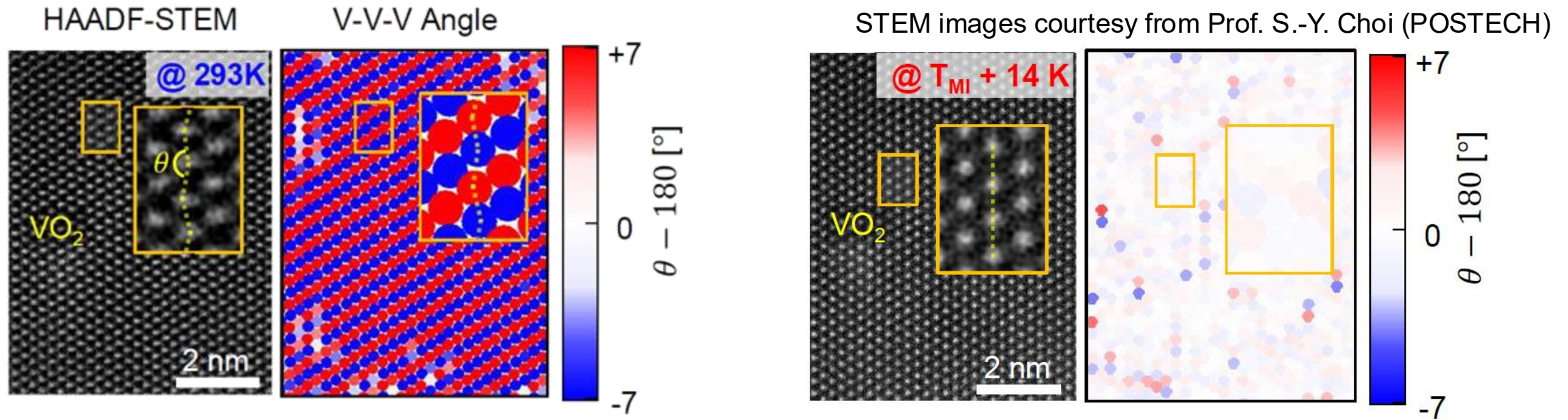
*Department of Physics, State University of New York at Stony Brook, Stony Brook, New York 11794-3800*

(Received 24 November 1993)

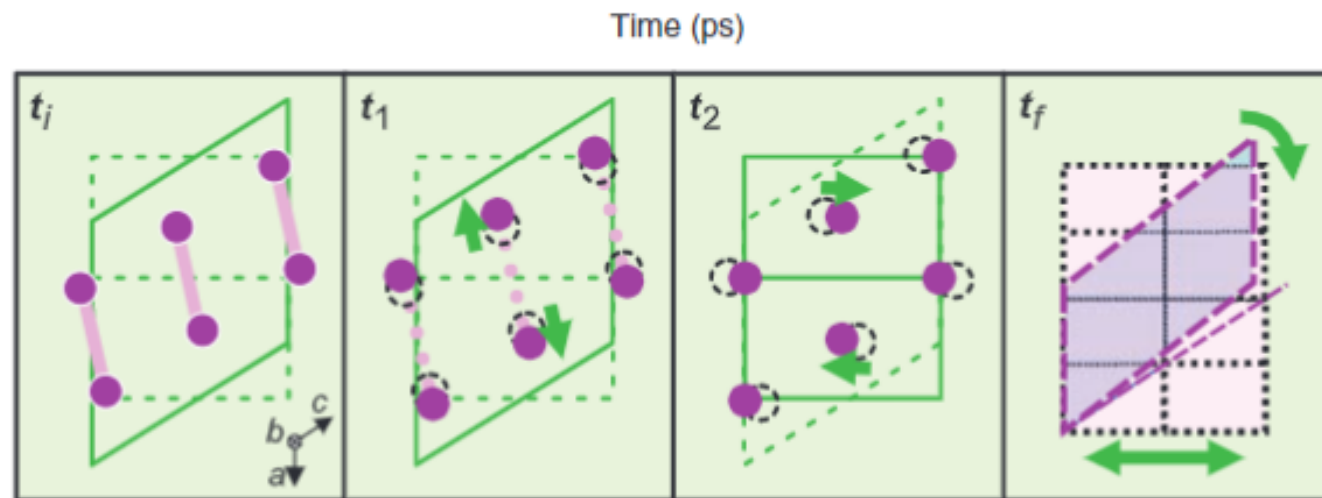
The electronic and structural properties of VO<sub>2</sub> across its metal-insulator transition are studied using the local-density approximation. Band theory finds a monoclinic distorted ground state in good agreement with experiment, and an almost open gap to charge excitations. Although rigid criteria for distinguishing correlated from band insulators are not available, these findings suggest that VO<sub>2</sub> may be more bandlike than correlated.

PACS numbers: 71.30.+h, 61.50.Ks, 71.25.Tn

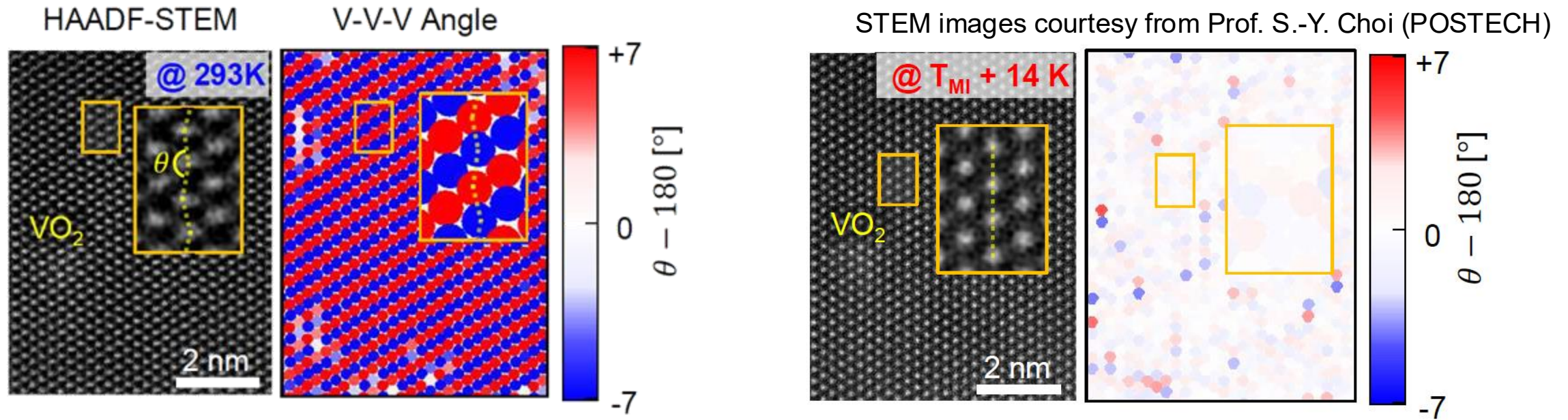
# Limitation of the structural transition



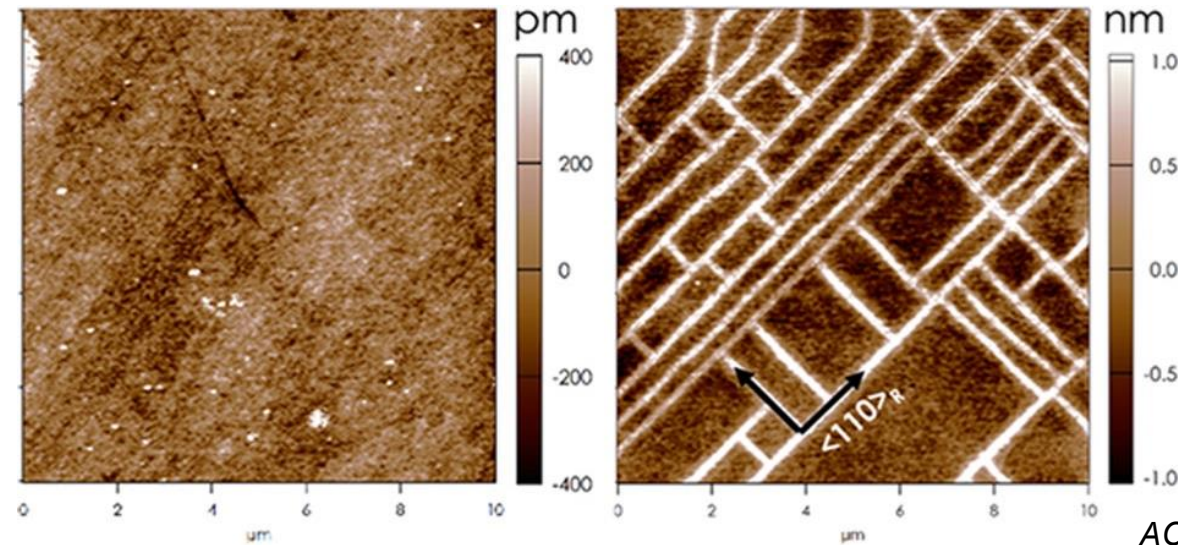
1. Atomic displacement on the sub-ns time scale



# Limitation of the structural transition

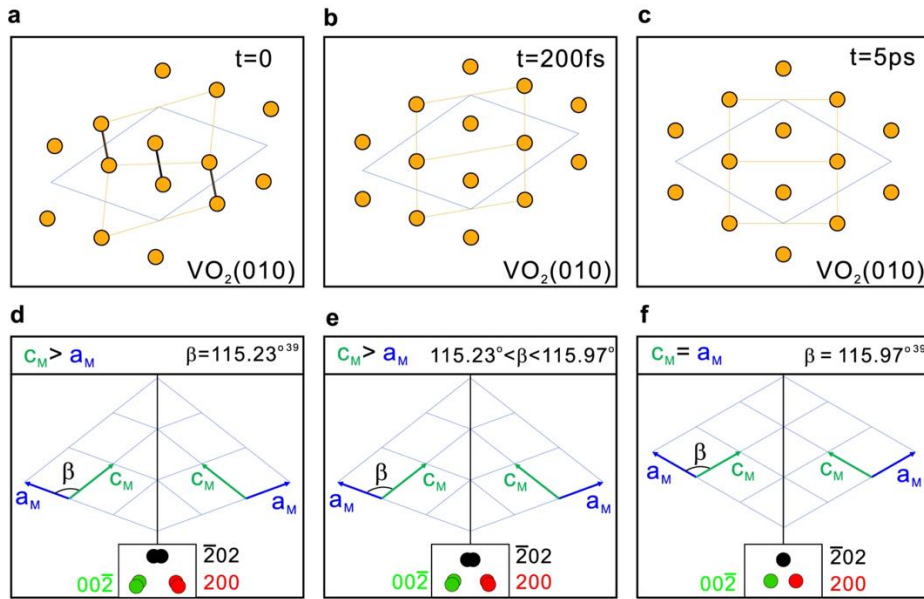


## 2. Microstructural crack generation

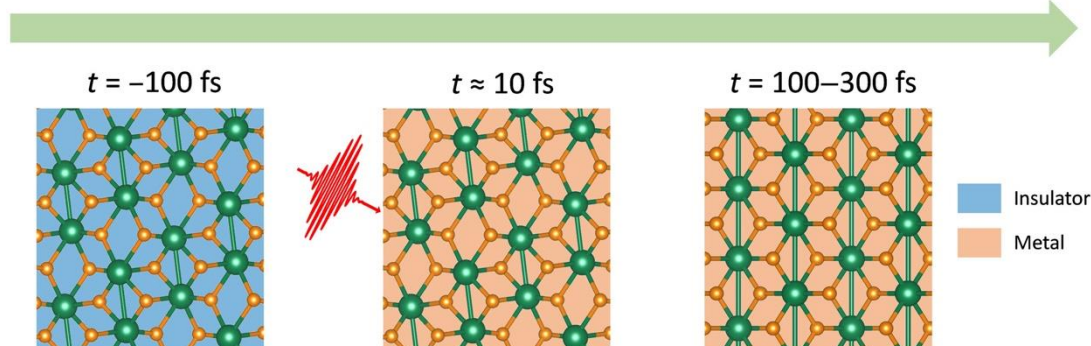


# Emergence of a metastable phase

## □ Light-induced metastable phase

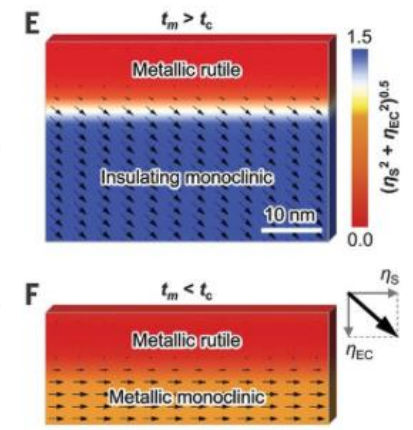
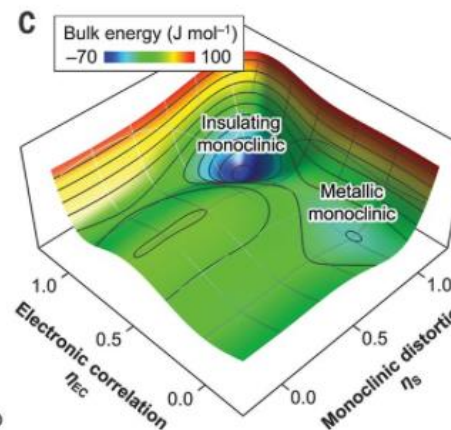
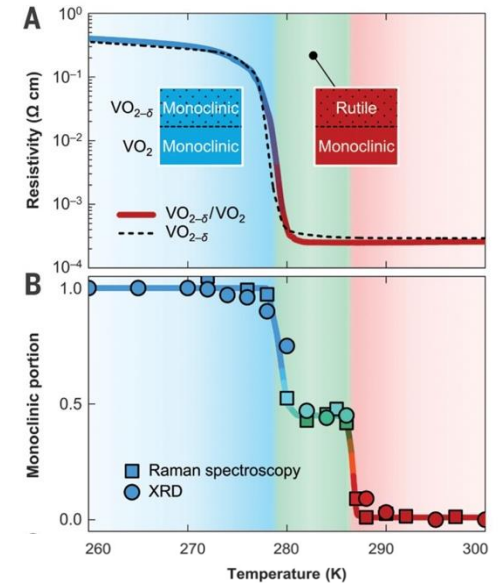
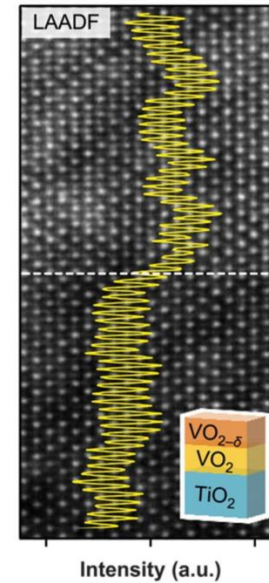


Nat. Commun 14, 1265 (2023)



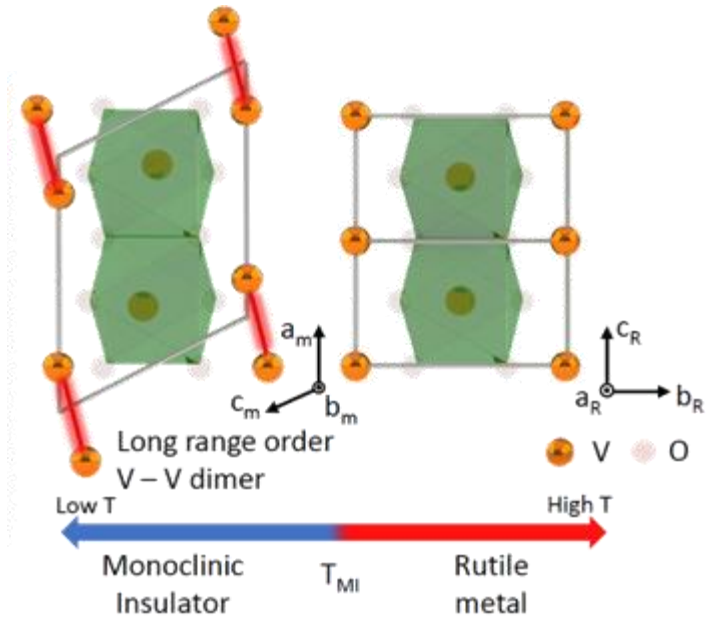
Nat. Commun 14, 1265 (2023)

## □ Heterostructure

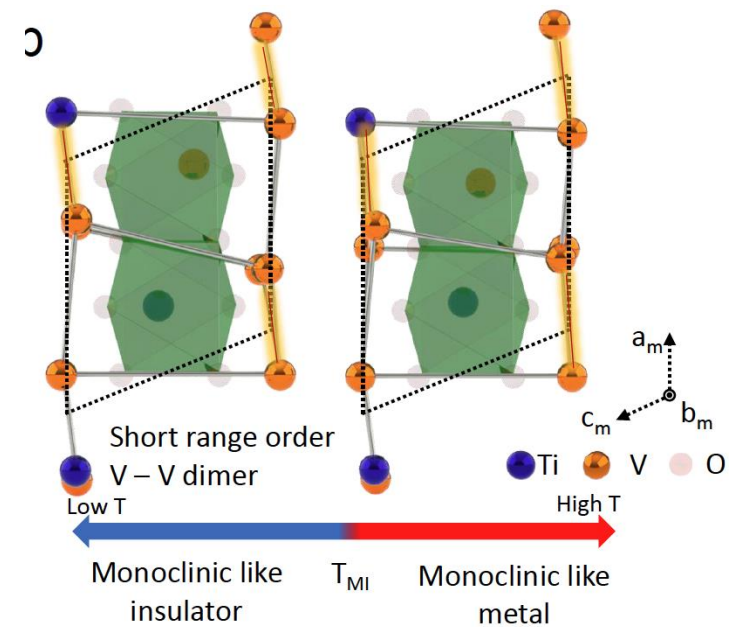


Science 362, 1037-1040 (2018)

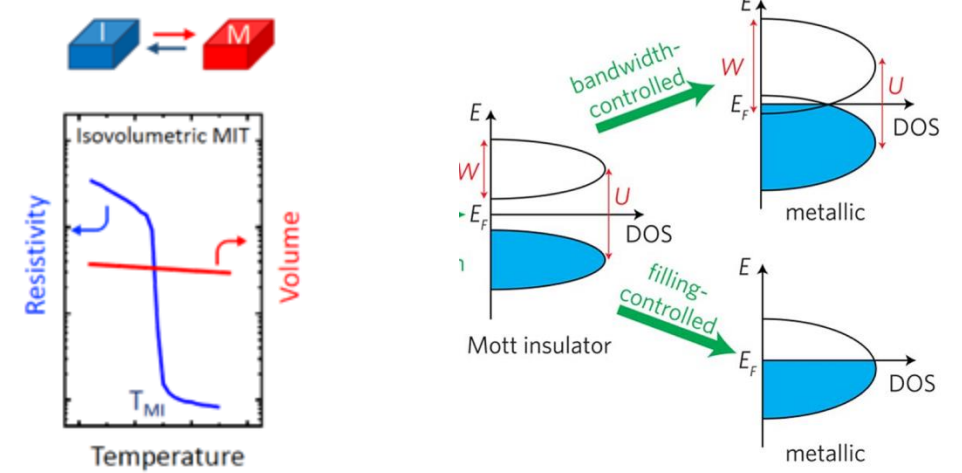
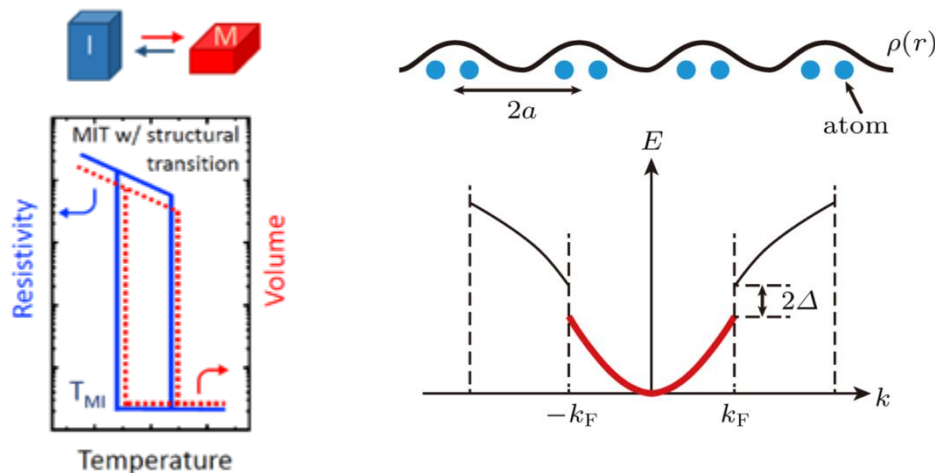
# Hypothesis for zero-strain metal insulator transition



Peierls distortion

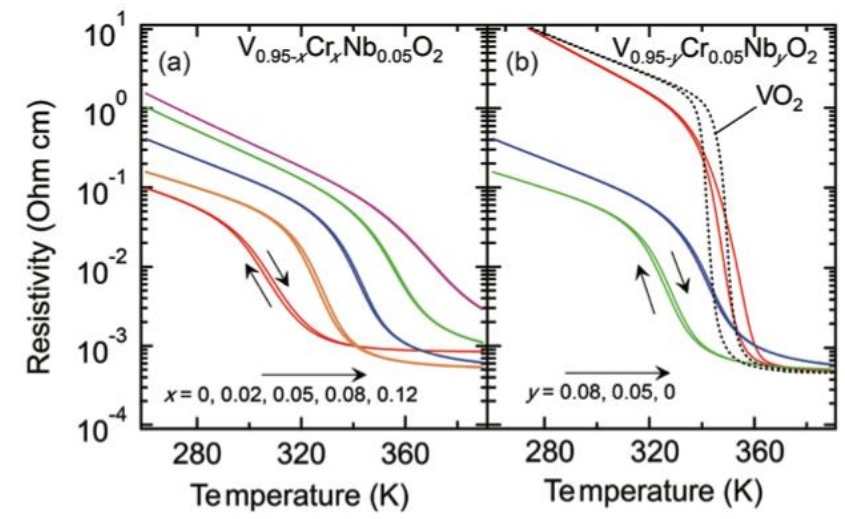
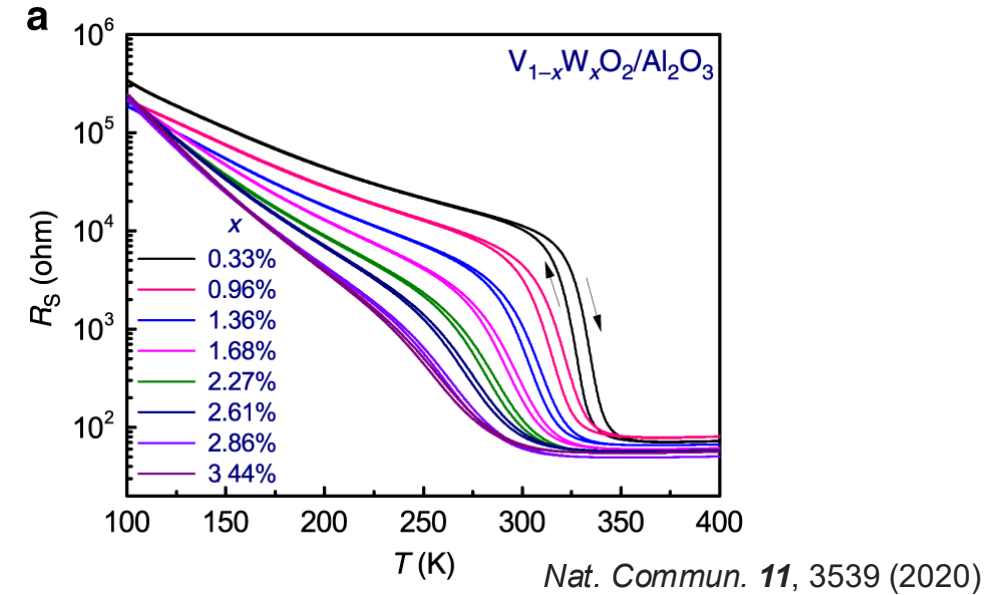


Mott like transition



# Exploring potential candidates for doping

		Rydberg constant		$R_\infty$		$10\,973\,731.569\text{ m}^{-1}$			
		Boltzmann constant		$R_\infty c$		$3.289\,841\,960 \times 10^{15}\text{ Hz}$			
				$R_\infty hc$		$13.605\,69\text{ eV}$			
				$k$		$1.380\,6 \times 10^{-23}\text{ J K}^{-1}$			
		3	4	5	6	7	8	9	
		IIIB	IVB	VB	VIB	VIIB	VIII		
3	11 <sup>2</sup> S <sub>1/2</sub> Na Sodium 22.989769 [Ne]3s <sup>1</sup> 5.1391	12 <sup>1</sup> S <sub>0</sub> Mg Magnesium 24.3050 [Ne]3s <sup>2</sup> 7.6462							
3d	19 <sup>2</sup> S <sub>1/2</sub> K Potassium 39.0983 [Ar]4s <sup>1</sup> 4.3407	20 <sup>1</sup> S <sub>0</sub> Ca Calcium 40.078 [Ar]4s <sup>2</sup> 6.1132	21 <sup>1</sup> D <sub>3/2</sub> Sc Scandium 44.955912 [Ar]3d <sup>1</sup> 4s <sup>2</sup>	22 <sup>1</sup> F <sub>2</sub> Ti Titanium 47.867 [Ar]3d <sup>2</sup> 4s <sup>2</sup> 6.8281	23 <sup>1</sup> F <sub>3/2</sub> V Vanadium 50.9415 [Ar]3d <sup>3</sup> 4s <sup>2</sup> 6.7462	24 <sup>1</sup> S <sub>3</sub> Cr Chromium 51.9961 [Ar]3d <sup>4</sup> 4s <sup>2</sup> 6.7665	25 <sup>5</sup> S <sub>5/2</sub> Mn Manganese 54.938045 [Ar]3d <sup>5</sup> 4s <sup>2</sup> 7.4340	26 <sup>1</sup> D <sub>3/2</sub> Fe Iron 55.845 [Ar]3d <sup>6</sup> 4s <sup>2</sup> 7.9025	27 <sup>1</sup> F <sub>5/2</sub> Co Cobalt 58.933195 [Ar]3d <sup>7</sup> 4s <sup>2</sup> 7.8810
4d	37 <sup>2</sup> S <sub>1/2</sub> Rb Rubidium 85.4678 [Kr]5s <sup>1</sup> 4.1771	38 <sup>1</sup> S <sub>0</sub> Sr Strontium 87.62 [Kr]5s <sup>2</sup> 5.6949	39 <sup>2</sup> D <sub>3/2</sub> Y Yttrium 88.90585 [Kr]4d <sup>5</sup> 5s <sup>2</sup> 6.2173	40 <sup>3</sup> F <sub>2</sub> Zr Zirconium 91.224 [Kr]4d <sup>2</sup> 5s <sup>2</sup> 6.6339	41 <sup>5</sup> D <sub>1/2</sub> Nb Niobium 92.90638 [Kr]4d <sup>4</sup> 5s 6.7589	42 <sup>7</sup> S <sub>3</sub> Mo Molybdenum 95.96 [Kr]4d <sup>5</sup> 5s 7.0924	43 <sup>6</sup> S <sub>5/2</sub> Tc Technetium (98) [Kr]4d <sup>5</sup> 5s <sup>2</sup> 7.1194	44 <sup>5</sup> F <sub>5</sub> Ru Ruthenium 101.07 [Kr]4d <sup>7</sup> 5s 7.3605	45 <sup>1</sup> F <sub>5/2</sub> Rh Rhodium 102.90550 [Kr]4d <sup>8</sup> 5s 7.4589
5d	55 <sup>1</sup> S <sub>1/2</sub> Cs Cesium 132.9054519 [Xe]6s <sup>1</sup> 3.8939	56 <sup>1</sup> S <sub>0</sub> Ba Barium 137.327 [Xe]6s <sup>2</sup> 5.2117	72 <sup>3</sup> F <sub>2</sub> Hf Hafnium 178.49 [Xe]4f <sup>14</sup> 5d <sup>2</sup> 6s <sup>2</sup> 6.8251	73 <sup>4</sup> F <sub>3/2</sub> Ta Tantalum 180.94788 [Xe]4f <sup>14</sup> 5d <sup>3</sup> 6s <sup>2</sup> 7.6496	74 <sup>5</sup> D <sub>0</sub> W Tungsten 183.84 [Xe]4f <sup>14</sup> 5d <sup>4</sup> 6s <sup>2</sup> 7.8640	75 <sup>6</sup> S <sub>5/2</sub> Re Rhenium 186.207 [Xe]4f <sup>14</sup> 5d <sup>5</sup> 6s <sup>2</sup> 7.8335	76 <sup>5</sup> D <sub>4</sub> Os Osmium 190.23 [Xe]4f <sup>14</sup> 5d <sup>6</sup> 6s <sup>2</sup> 8.4382	77 <sup>1</sup> F <sub>5/2</sub> Ir Iridium 192.217 [Xe]4f <sup>14</sup> 5d <sup>7</sup> 6s <sup>2</sup> 8.9670	
7	104 <sup>1</sup> F <sub>2</sub> Rf Rutherfordium (261) [Rn]5f <sup>14</sup> 6d <sup>2</sup> 7s <sup>2</sup> 6.01	105 <sup>1</sup> F <sub>3/2</sub> Db Dubnium (268) [Rn]5f <sup>14</sup> 6d <sup>3</sup> 7s <sup>2</sup> 6.8	106 <sup>1</sup> F <sub>3/2</sub> Sg Seaborgium (271) [Rn]5f <sup>14</sup> 6d <sup>4</sup> 7s <sup>2</sup> 7.8	107 <sup>1</sup> F <sub>3/2</sub> Bh Bohrium (270) [Rn]5f <sup>14</sup> 6d <sup>5</sup> 7s <sup>2</sup> 7.7	108 <sup>1</sup> F <sub>3/2</sub> Hs Hassium (277) [Rn]5f <sup>14</sup> 6d <sup>6</sup> 7s <sup>2</sup> 7.6	109 <sup>1</sup> F <sub>3/2</sub> Mt Meitnerium (276) [Rn]5f <sup>14</sup> 6d <sup>7</sup> 7s <sup>2</sup>			

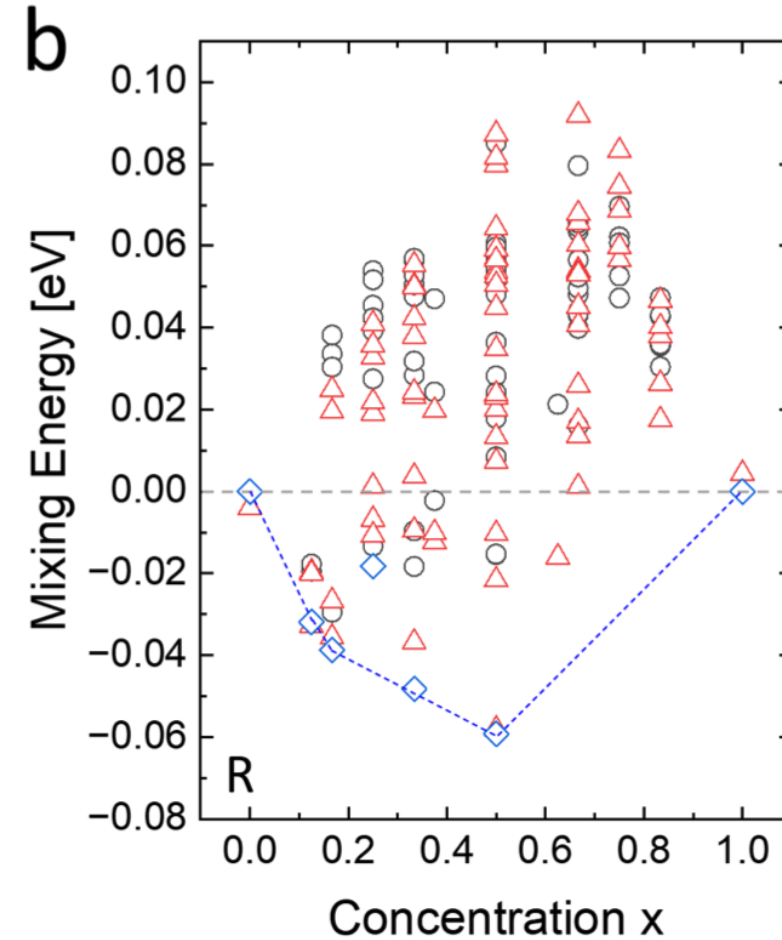
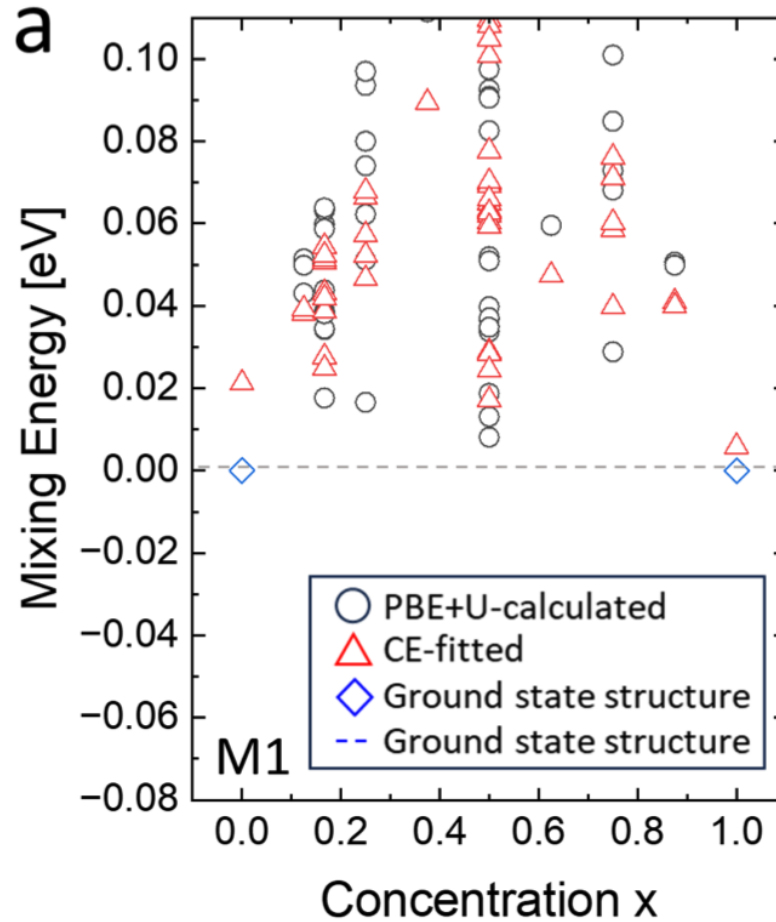


# Exploring potential candidates for doping

		Rydberg constant																		
		$R_{\infty}$										$10\,973\,731.569\text{ m}^{-1}$								
		$R_{\infty}c$										$3.289\,841\,960 \times 10^{15}\text{ Hz}$								
		$R_{\infty}hc$										$13.605\,69\text{ eV}$								
		Boltzmann constant										$k$								
		$1.380\,6 \times 10^{-23}\text{ J K}^{-1}$																		
		11 <sup>3s</sup> <sub>1/2</sub> <b>Na</b> Sodium 22.98976928 [Ne]3s 5.1391	12 <sup>3s</sup> <sub>3/2</sub> <b>Mg</b> Magnesium 24.304 [Ne] 7.6												13 <sup>3p</sup> <sub>1/2</sub> <b>Al</b> Aluminum 26.9815386 [Ne]3s <sup>2</sup> 3p 5.9858	14 <sup>3p</sup> <sub>3/2</sub> <b>Si</b> Silicon 28.085 [Ne]3s <sup>2</sup> 3p <sup>2</sup> 8.1517	15 <sup>3s</sup> <sub>3/2</sub> <b>P</b> Phosphorus 30.973762 [Ne]3s <sup>2</sup> 3p <sup>3</sup> 10.4867	16 <sup>3p</sup> <sub>3/2</sub> <b>S</b> Sulfur 32.06 [Ne]3s <sup>2</sup> 3p <sup>4</sup> 10.3600	17 <sup>3p</sup> <sub>3/2</sub> <b>Cl</b> Chlorine 35.45 [Ne]3s <sup>2</sup> 3p <sup>5</sup> 12.9676	18 <sup>3s</sup> <sub>3/2</sub> <b>Ar</b> Argon 39.948 [Ne]3s <sup>2</sup> 3p <sup>6</sup> 15.7596
				4 IIB	5 VB	6 VIB	7 VIIB	8 VIII	9 VIII	10 VIII	11 IB	12 IIB								
3d		19 <sup>3d</sup> <sub>3/2</sub> <b>K</b> Potassium 39.0983 [Ar]4s 4.3407	20 <sup>3d</sup> <sub>5/2</sub> <b>Ca</b> Calcium 40.078 [Ar]4s <sup>2</sup> 6.1132	21 <sup>3d</sup> <sub>5/2</sub> <b>Sc</b> Scandium 44.955912 [Ar]3d <sup>1</sup> 4s <sup>2</sup> 6.5615	22 <sup>3d</sup> <sub>3/2</sub> <b>Ti</b> Titanium 47.867 [Ar]3d <sup>2</sup> 4s <sup>2</sup> 6.8281	23 <sup>3d</sup> <sub>5/2</sub> <b>V</b> Vanadium 50.9415 [Ar]3d <sup>3</sup> 4s <sup>2</sup> 6.7462	24 <sup>3d</sup> <sub>5/2</sub> <b>Cr</b> Chromium 51.9961 [Ar]3d <sup>5</sup> 4s 8.7865	25 <sup>3d</sup> <sub>5/2</sub> <b>Mn</b> Manganese 54.938045 [Ar]3d <sup>5</sup> 4s <sup>2</sup> 7.4340	26 <sup>3d</sup> <sub>5/2</sub> <b>Fe</b> Iron 55.845 [Ar]3d <sup>6</sup> 4s <sup>2</sup> 7.9025	27 <sup>3d</sup> <sub>5/2</sub> <b>Co</b> Cobalt 58.933195 [Ar]3d <sup>7</sup> 4s <sup>2</sup> 7.8810	28 <sup>3d</sup> <sub>5/2</sub> <b>Ni</b> Nickel 58.6934 [Ar]3d <sup>8</sup> 4s <sup>2</sup> 7.6399	29 <sup>3d</sup> <sub>5/2</sub> <b>Cu</b> Copper 63.546 [Ar]3d <sup>10</sup> 4s 7.7264	30 <sup>3d</sup> <sub>5/2</sub> <b>Zn</b> Zinc 65.38 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 9.3942	31 <sup>3d</sup> <sub>5/2</sub> <b>Ga</b> Gallium 69.723 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p 5.9993	32 <sup>3p</sup> <sub>3/2</sub> <b>Ge</b> Germanium 72.63 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>2</sup> 7.8994	33 <sup>3s</sup> <sub>3/2</sub> <b>As</b> Arsenic 74.92160 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>3</sup> 9.7886	34 <sup>3p</sup> <sub>3/2</sub> <b>Se</b> Selenium 78.96 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>4</sup> 9.7524	35 <sup>3p</sup> <sub>3/2</sub> <b>Br</b> Bromine 79.904 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>5</sup> 11.8138	36 <sup>3s</sup> <sub>3/2</sub> <b>Kr</b> Krypton 83.798 [Ar]3d <sup>10</sup> 4s <sup>2</sup> 4p <sup>6</sup> 13.9996	
4d		37 <sup>4d</sup> <sub>3/2</sub> <b>Rb</b> Rubidium 85.4678 [Kr]5s 4.1771	38 <sup>4d</sup> <sub>5/2</sub> <b>Sr</b> Strontium 87.62 [Kr]5s <sup>2</sup> 5.6949	39 <sup>4d</sup> <sub>5/2</sub> <b>Y</b> Yttrium 88.90585 [Kr]4d <sup>1</sup> 5s <sup>2</sup> 6.2173	40 <sup>4d</sup> <sub>3/2</sub> <b>Zr</b> Zirconium 91.224 [Kr]4d <sup>2</sup> 5s <sup>2</sup> 6.6339	41 <sup>4d</sup> <sub>5/2</sub> <b>Nb</b> Niobium 92.90638 [Kr]4d <sup>4</sup> 5s 6.7589	42 <sup>4d</sup> <sub>3/2</sub> <b>Mo</b> Molybdenum 95.96 [Kr]4d <sup>5</sup> 5s 7.0924	43 <sup>4d</sup> <sub>3/2</sub> <b>Tc</b> Technetium (98) [Kr]4d <sup>5</sup> 5s <sup>2</sup> 7.1194	44 <sup>4d</sup> <sub>3/2</sub> <b>Ru</b> Ruthenium 101.07 [Kr]4d <sup>7</sup> 5s 7.3605	45 <sup>4d</sup> <sub>3/2</sub> <b>Rh</b> Rhodium 102.90550 [Kr]4d <sup>8</sup> 5s 7.4589	46 <sup>4d</sup> <sub>3/2</sub> <b>Pd</b> Palladium 106.42 [Kr]4d <sup>10</sup> 8.3369	47 <sup>4d</sup> <sub>3/2</sub> <b>Ag</b> Silver 107.8682 [Kr]4d <sup>10</sup> 5s 7.5762	48 <sup>4d</sup> <sub>3/2</sub> <b>Cd</b> Cadmium 112.411 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p 8.9938	49 <sup>4d</sup> <sub>3/2</sub> <b>In</b> Indium 114.818 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>2</sup> 5.7864	50 <sup>4d</sup> <sub>3/2</sub> <b>Sn</b> Tin 118.710 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>3</sup> 7.3439	51 <sup>4d</sup> <sub>3/2</sub> <b>Sb</b> Antimony 121.760 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>3</sup> 8.6084	52 <sup>4d</sup> <sub>3/2</sub> <b>Te</b> Tellurium 127.60 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>4</sup> 9.0097	53 <sup>4d</sup> <sub>3/2</sub> <b>I</b> Iodine 126.90447 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>5</sup> 10.4513	54 <sup>4d</sup> <sub>3/2</sub> <b>Xe</b> Xenon 131.293 [Kr]4d <sup>10</sup> 5s <sup>2</sup> 5p <sup>6</sup> 12.1298	
5d		55 <sup>5d</sup> <sub>3/2</sub> <b>Cs</b> Cesium 132.9054519 [Xe]6s 3.8939	56 <sup>5d</sup> <sub>5/2</sub> <b>Ba</b> Barium 137.327 [Xe]6s <sup>2</sup> 5.2117		72 <sup>5d</sup> <sub>3/2</sub> <b>Hf</b> Hafnium 178.49 [Xe]4f <sup>14</sup> 5d <sup>2</sup> 6s <sup>2</sup> 6.8251	73 <sup>5d</sup> <sub>5/2</sub> <b>Ta</b> Tantalum 180.94788 [Xe]4f <sup>14</sup> 5d <sup>3</sup> 6s <sup>2</sup> 7.5496	74 <sup>5d</sup> <sub>3/2</sub> <b>W</b> Tungsten 183.84 [Xe]4f <sup>14</sup> 5d <sup>4</sup> 6s <sup>2</sup> 7.8640	75 <sup>5d</sup> <sub>3/2</sub> <b>Re</b> Rhenium 186.207 [Xe]4f <sup>14</sup> 5d <sup>5</sup> 6s <sup>2</sup> 7.8335	76 <sup>5d</sup> <sub>3/2</sub> <b>Os</b> Osmium 190.23 [Xe]4f <sup>14</sup> 5d <sup>6</sup> 6s <sup>2</sup> 8.4382	77 <sup>5d</sup> <sub>3/2</sub> <b>Ir</b> Iridium 192.217 [Xe]4f <sup>14</sup> 5d <sup>7</sup> 6s <sup>2</sup> 8.9670	78 <sup>5d</sup> <sub>3/2</sub> <b>Pt</b> Platinum 195.084 [Xe]4f <sup>14</sup> 5d <sup>9</sup> 6s <sup>1</sup> 8.9588	79 <sup>5d</sup> <sub>3/2</sub> <b>Au</b> Gold 196.966569 [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>1</sup> 9.2256	80 <sup>5d</sup> <sub>3/2</sub> <b>Hg</b> Mercury 200.59 [Xe]4f <sup>14</sup> 5d <sup>10</sup> 6s <sup>2</sup> 10.4375	81 <sup>5d</sup> <sub>3/2</sub> <b>Tl</b> Thallium 204.38 [Hg]6p 6.1083	82 <sup>5d</sup> <sub>3/2</sub> <b>Pb</b> Lead 207.2 [Hg]6p <sup>2</sup> 7.4167	83 <sup>5d</sup> <sub>3/2</sub> <b>Bi</b> Bismuth 208.98040 [Hg]6p <sup>3</sup> 7.2855	84 <sup>5d</sup> <sub>3/2</sub> <b>Po</b> Polonium (209) [Hg]6p <sup>4</sup> 8.414	85 <sup>5d</sup> <sub>3/2</sub> <b>At</b> Astatine (210) [Hg]6p <sup>5</sup> 9.350	86 <sup>5d</sup> <sub>3/2</sub> <b>Rn</b> Radon (222) [Hg]6p <sup>6</sup> 10.7485	
7		87 <sup>7s</sup> <sub>1/2</sub> <b>Fr</b> Francium (223) [Rn]7s 4.0727	88 <sup>7s</sup> <sub>1/2</sub> <b>Ra</b> Radium (226) [Rn]7s <sup>2</sup> 5.2784		104 <sup>7s</sup> <sub>1/2</sub> <b>Rf</b> Rutherfordium (261) [Rn]5f <sup>14</sup> 6d <sup>2</sup> 7s <sup>2</sup> 6.01	105 <sup>7s</sup> <sub>3/2</sub> <b>Db</b> Dubnium (268) [Rn]5f <sup>14</sup> 6d <sup>3</sup> 7s <sup>2</sup> 6.8	106 <sup>7s</sup> <sub>3/2</sub> <b>Sg</b> Seaborgium (271) [Rn]5f <sup>14</sup> 6d <sup>4</sup> 7s <sup>2</sup> 7.8	107 <sup>7s</sup> <sub>3/2</sub> <b>Bh</b> Bohrium (270) [Rn]5f <sup>14</sup> 6d <sup>5</sup> 7s <sup>2</sup> 7.7	108 <sup>7s</sup> <sub>3/2</sub> <b>Hs</b> Hassium (277) [Rn]5f <sup>14</sup> 6d <sup>6</sup> 7s <sup>2</sup> 7.6	109 <sup>7s</sup> <sub>3/2</sub> <b>Mt</b> Meitnerium (276) [Rn]5f <sup>14</sup> 6d <sup>7</sup> 7s <sup>2</sup>	110 <sup>7s</sup> <sub>3/2</sub> <b>Ds</b> Darmstadtium (281) [Rn]5f <sup>14</sup> 6d <sup>8</sup> 7s <sup>2</sup>	111 <sup>7s</sup> <sub>3/2</sub> <b>Rg</b> Roentgenium (280) [Rn]5f <sup>14</sup> 6d <sup>9</sup> 7s <sup>2</sup>	112 <sup>7s</sup> <sub>3/2</sub> <b>Cn</b> Copernicium (285) [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup>	113 <sup>7s</sup> <sub>3/2</sub> <b>Uut</b> Ununtrium (284) [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>1</sup>	114 <sup>7s</sup> <sub>3/2</sub> <b>Fl</b> Flerovium (289) [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>2</sup>	115 <sup>7s</sup> <sub>3/2</sub> <b>Uup</b> Ununpentium (288) [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>3</sup>	116 <sup>7s</sup> <sub>3/2</sub> <b>Lv</b> Livermorium (293) [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>4</sup>	117 <sup>7s</sup> <sub>3/2</sub> <b>Uus</b> Ununseptium (294) [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>5</sup>	118 <sup>7s</sup> <sub>3/2</sub> <b>Uuo</b> Ununoctium (294) [Rn]5f <sup>14</sup> 6d <sup>10</sup> 7s <sup>2</sup> 7p <sup>6</sup>	

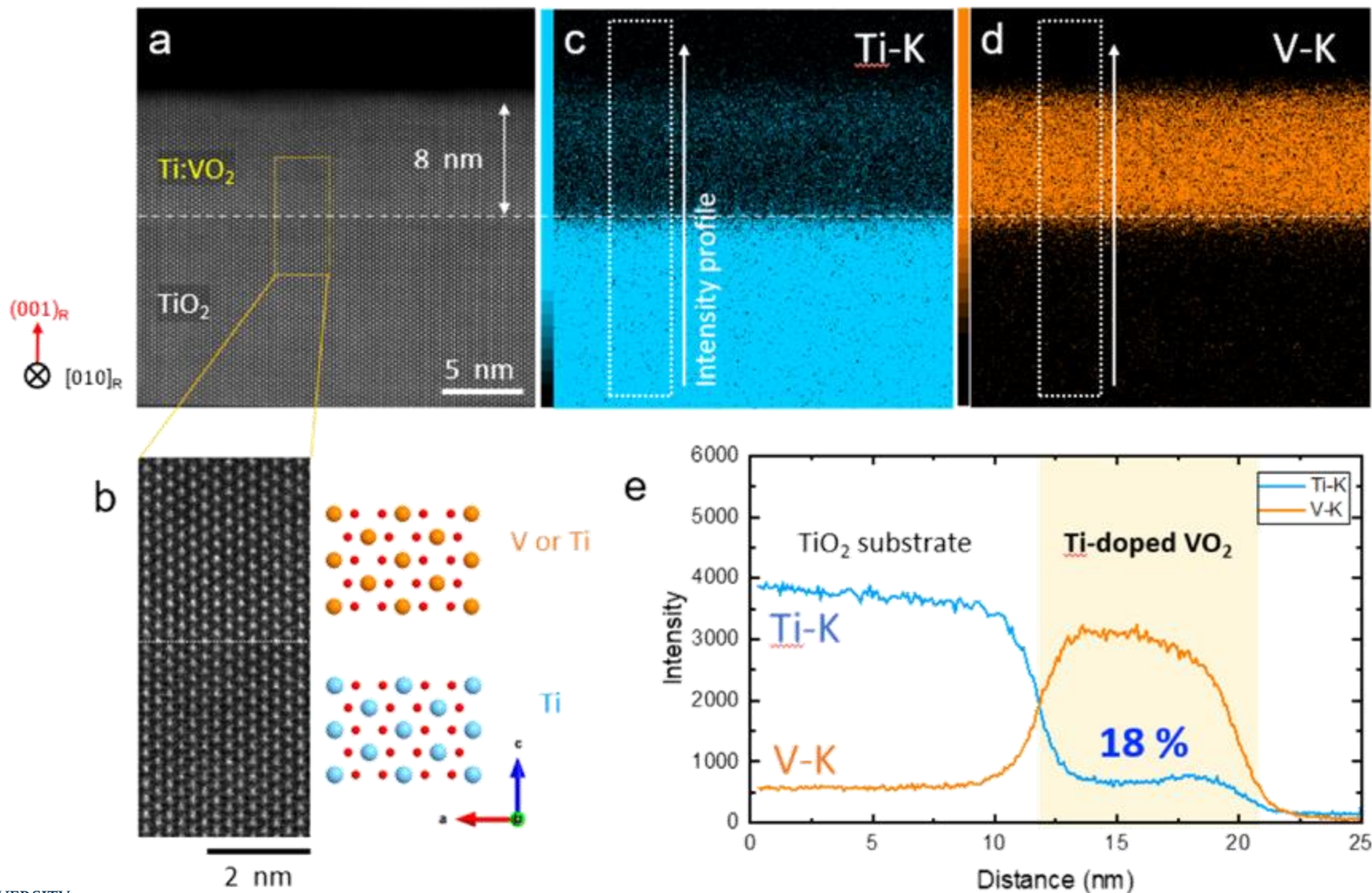
# Synthesis of Ti-doped $\text{VO}_2$

DFT calculation courtesy from Prof. J. K. Lee (PNU)

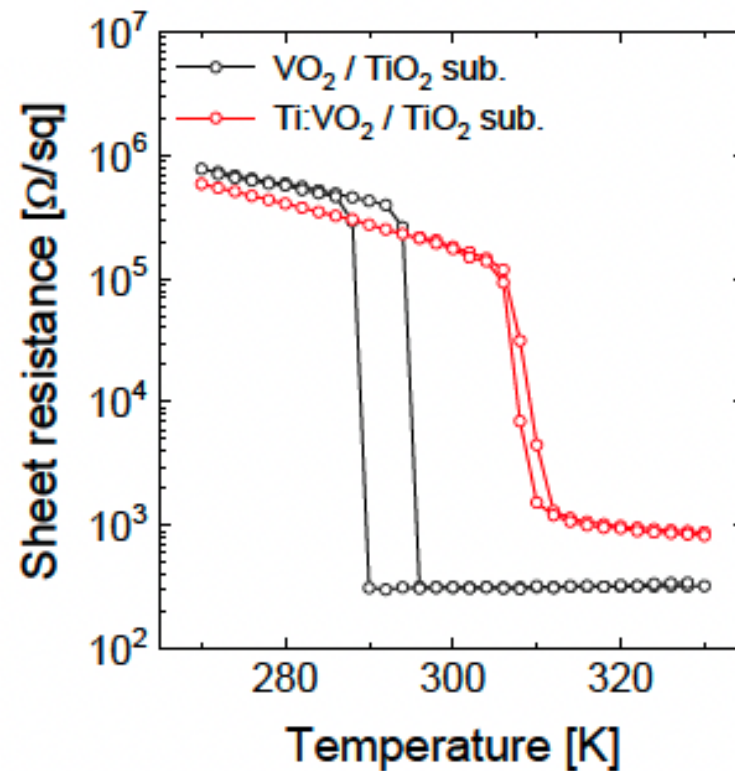
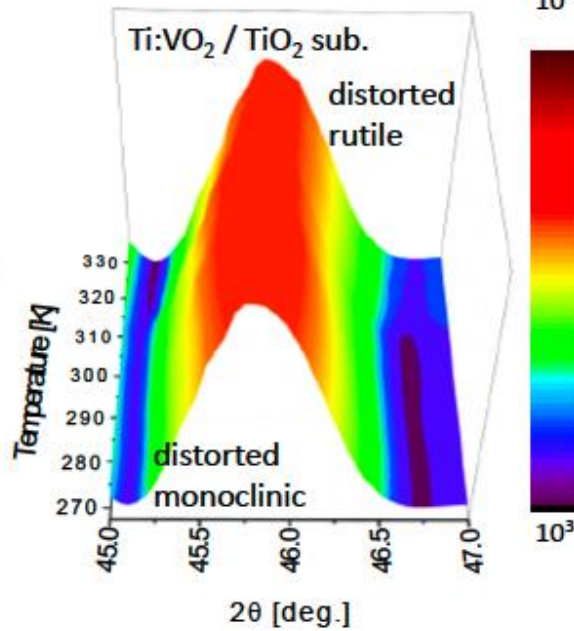
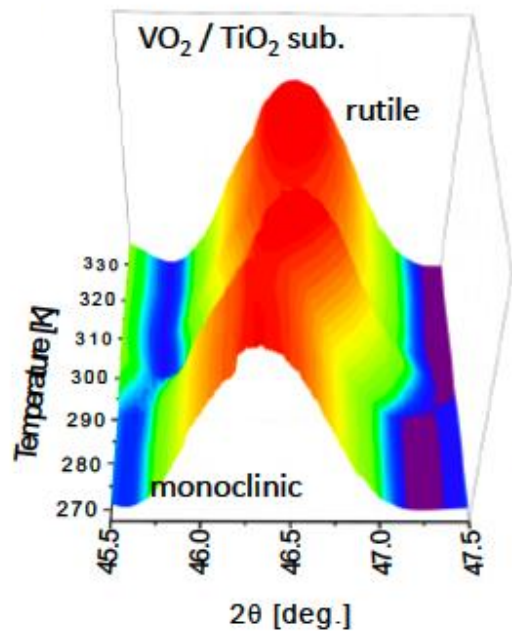
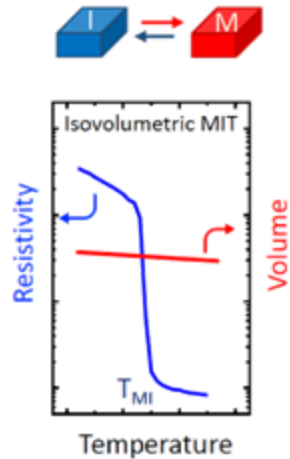
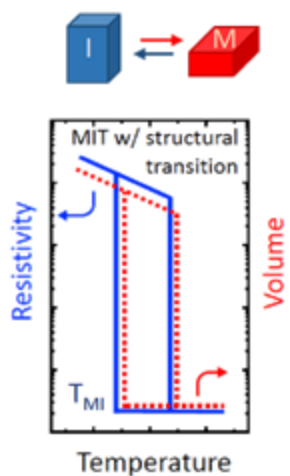


# Synthesis of Ti-doped VO<sub>2</sub>

STEM images courtesy from Prof. S.-Y. Choi (POSTECH)

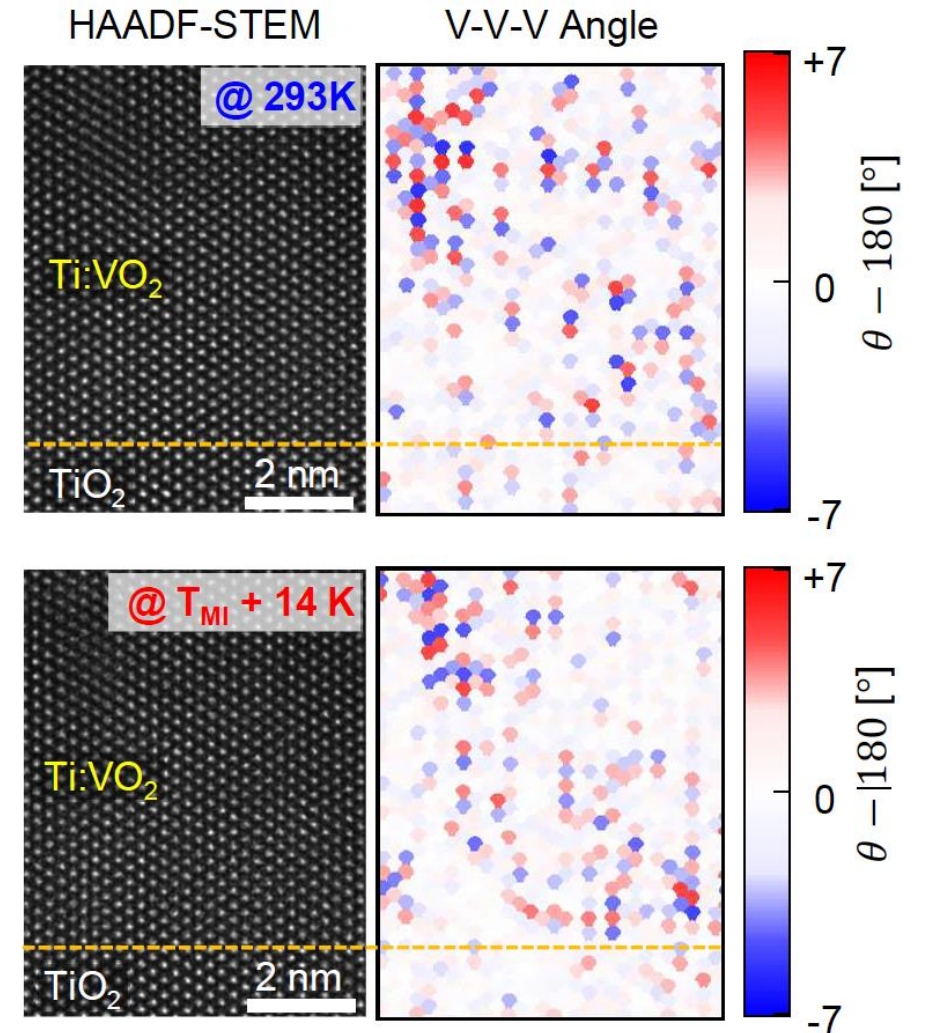
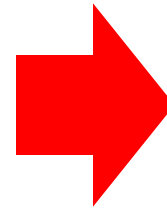
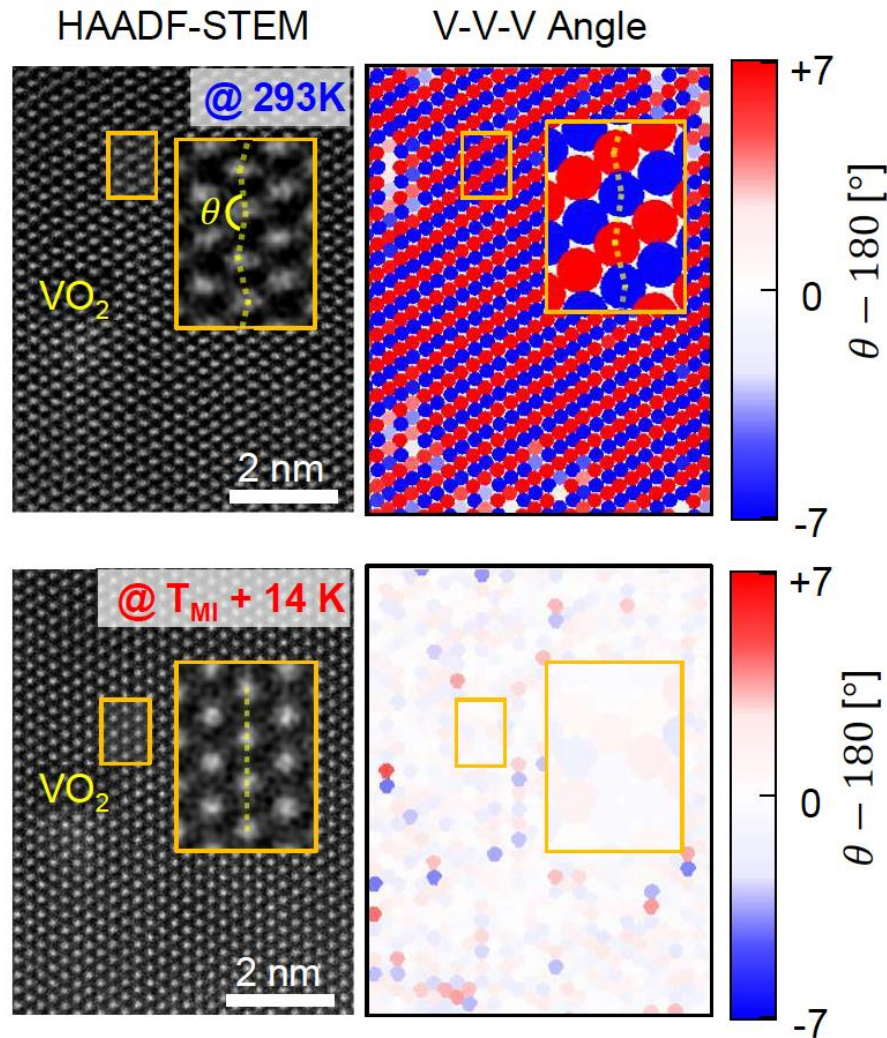


# Iso-volumetric phase transition



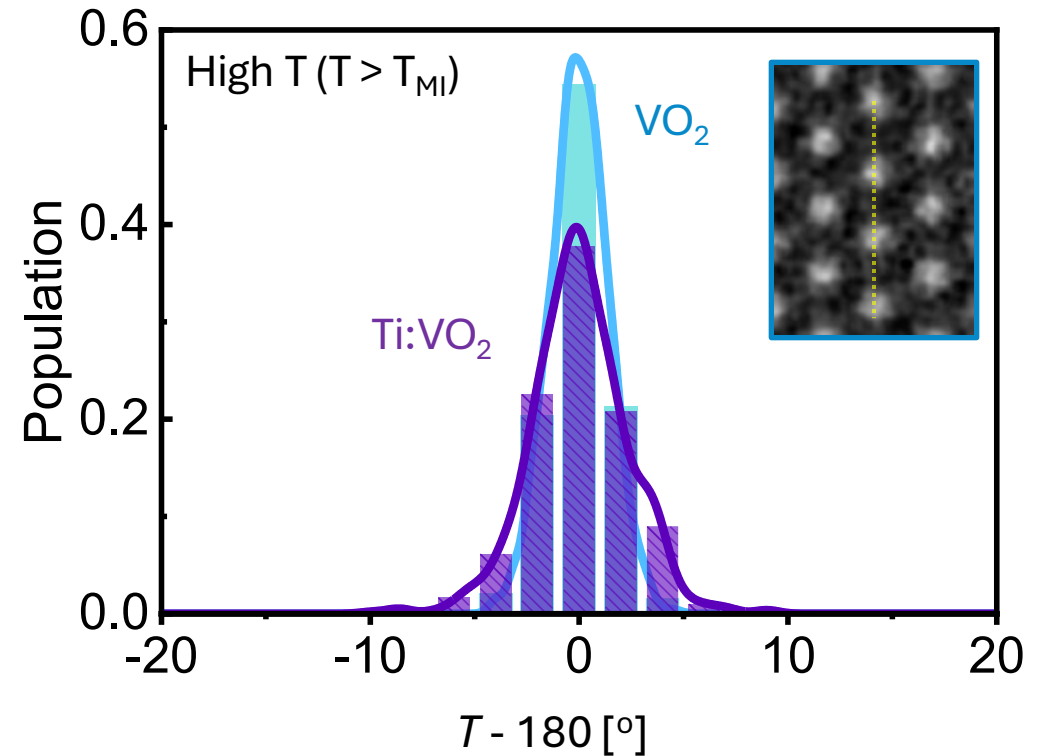
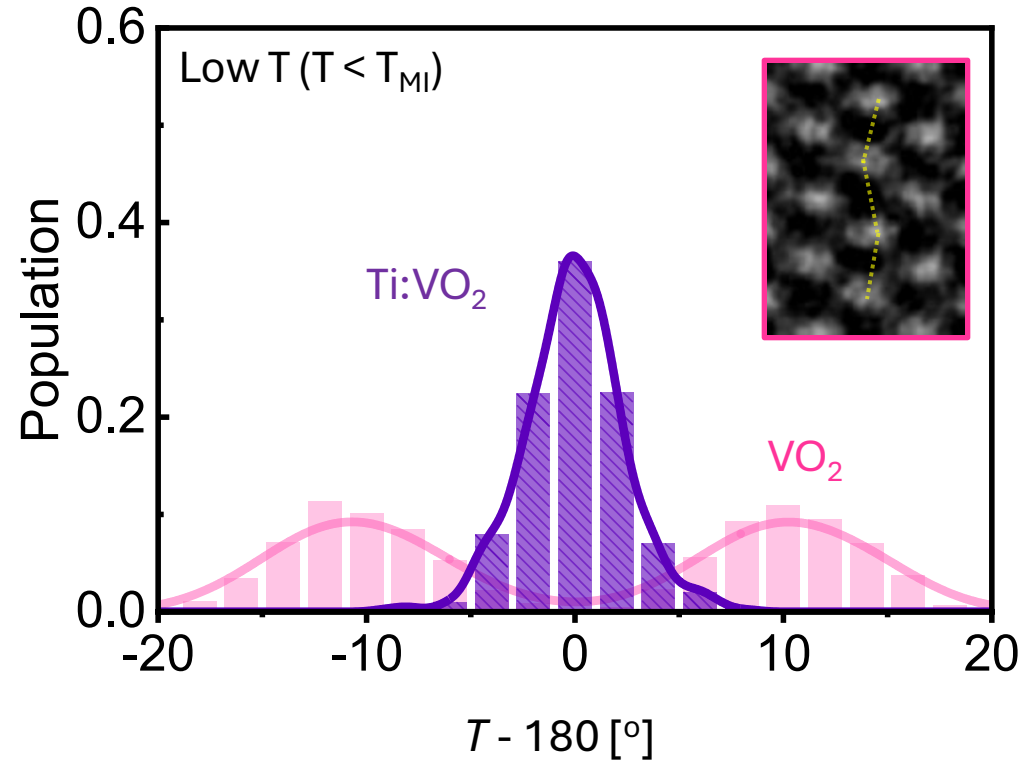
# Persistent V-V dimerization

STEM images courtesy from Prof. S.-Y. Choi (POSTECH)



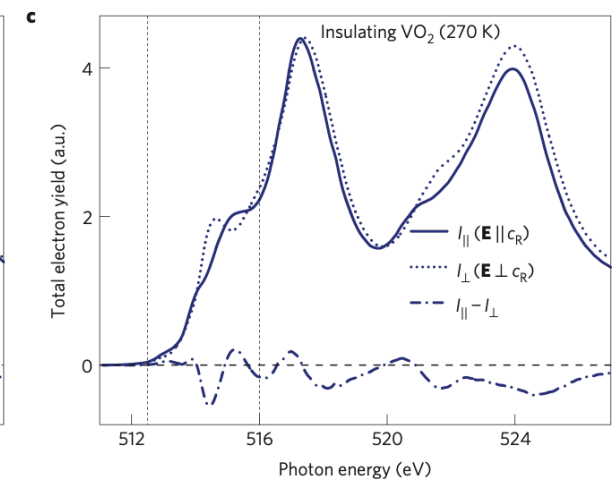
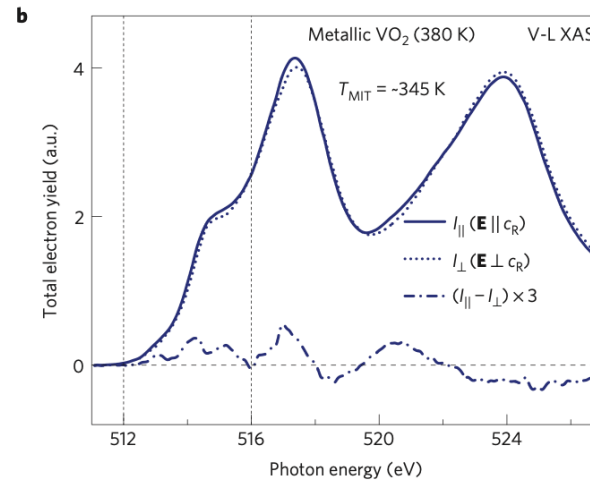
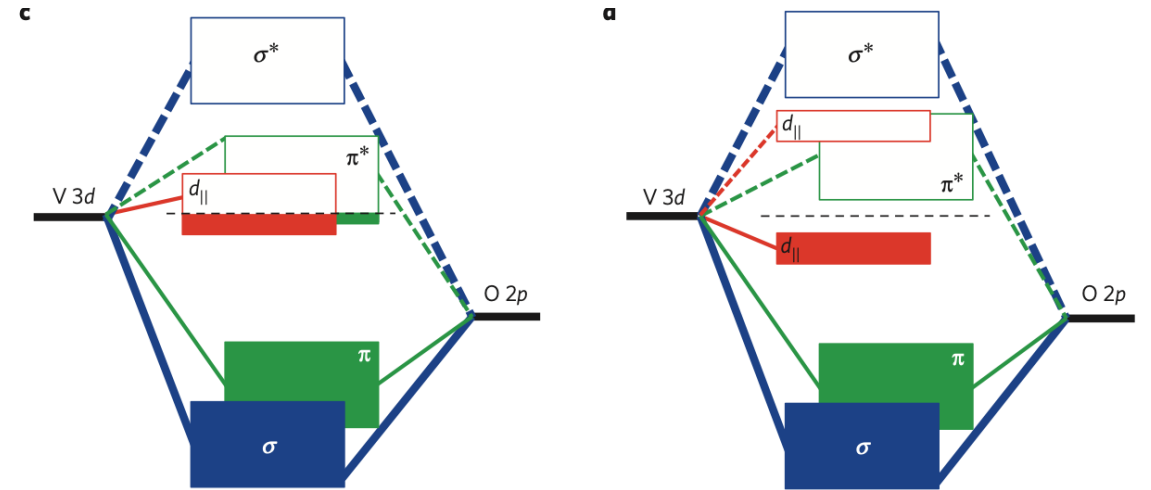
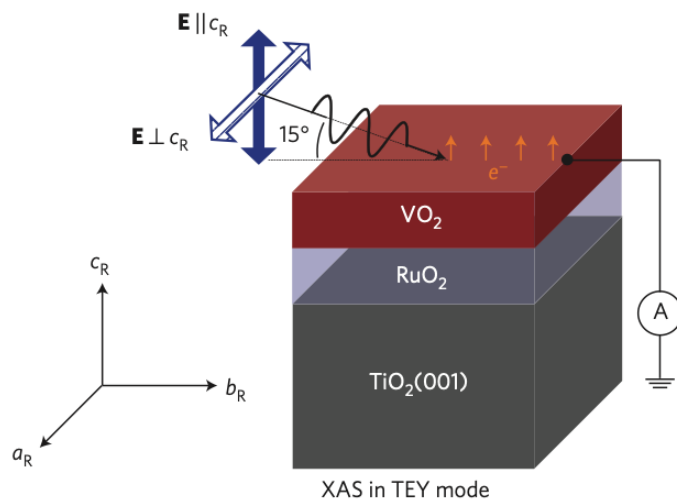
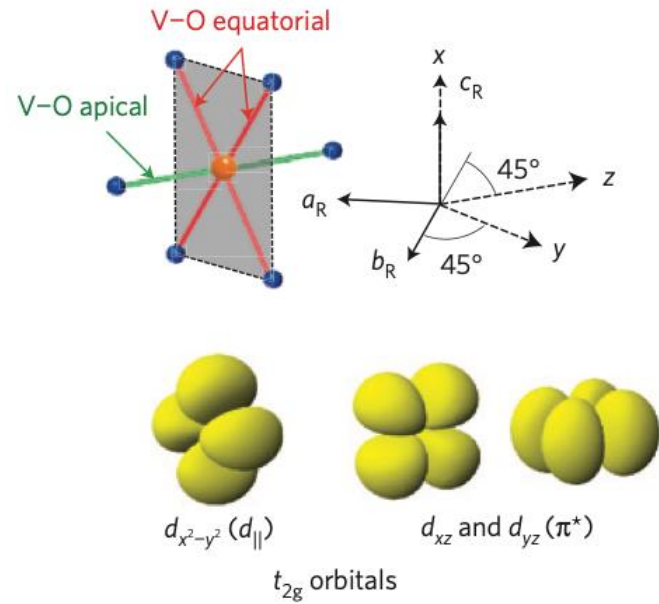
# Persistent V-V dimerization

STEM images courtesy from Prof. S.-Y. Choi (POSTECH)



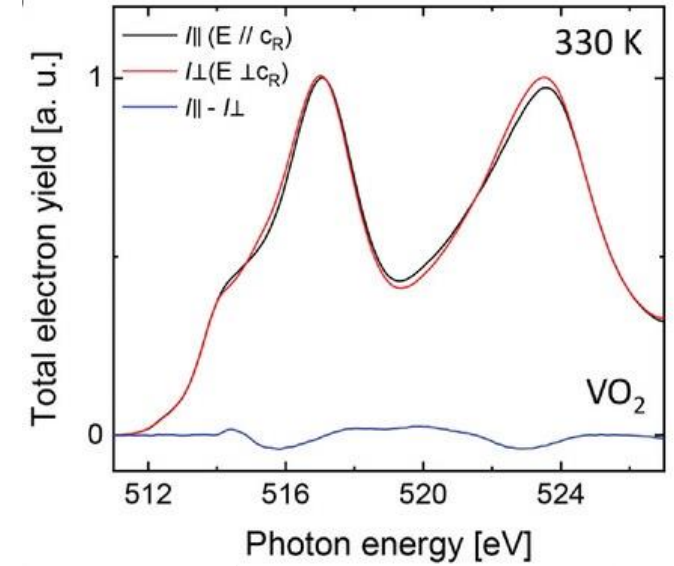
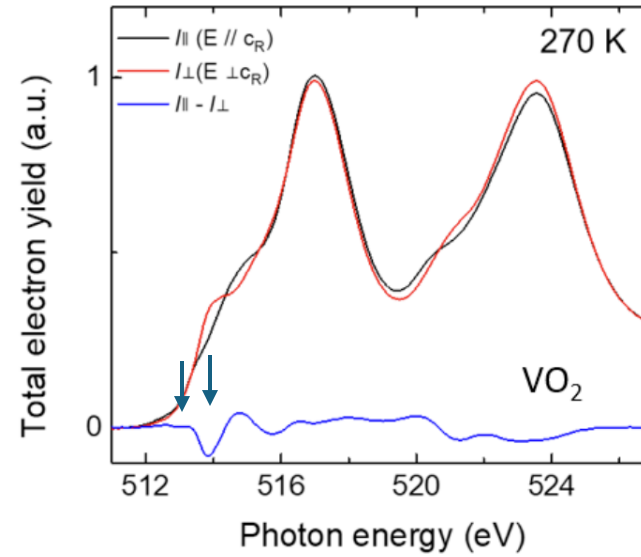
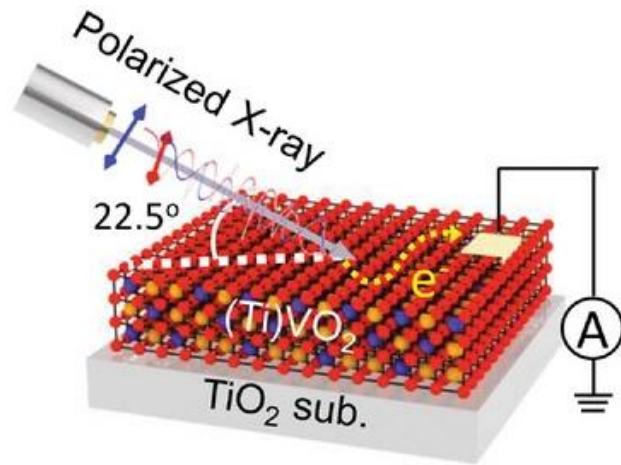
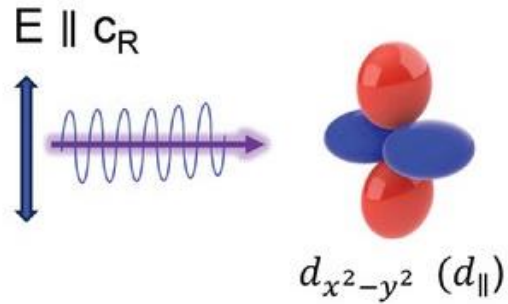
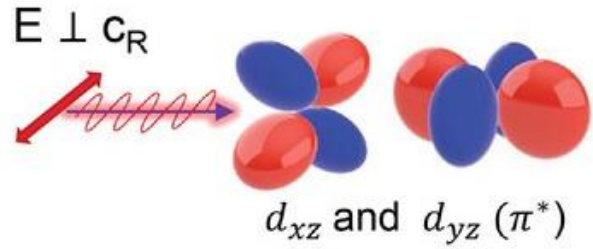
- Ti dopants in the VO<sub>2</sub> lattice locally alter the configuration of V-V pairs, where the long-range ordering in V-V pairs is disrupted.

# Polarization-dependent XAS

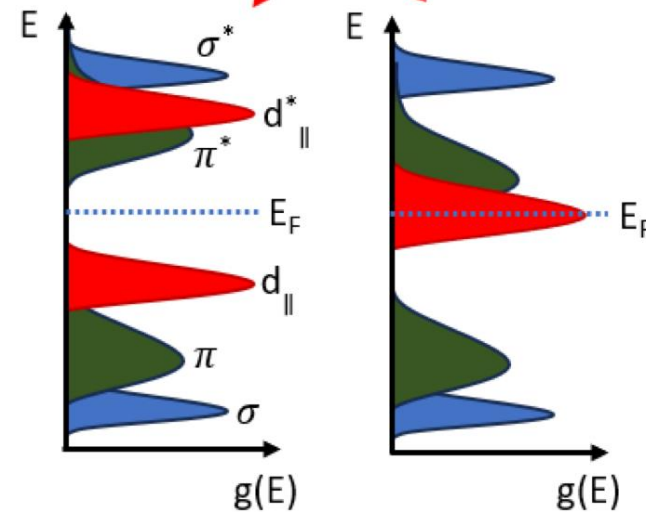


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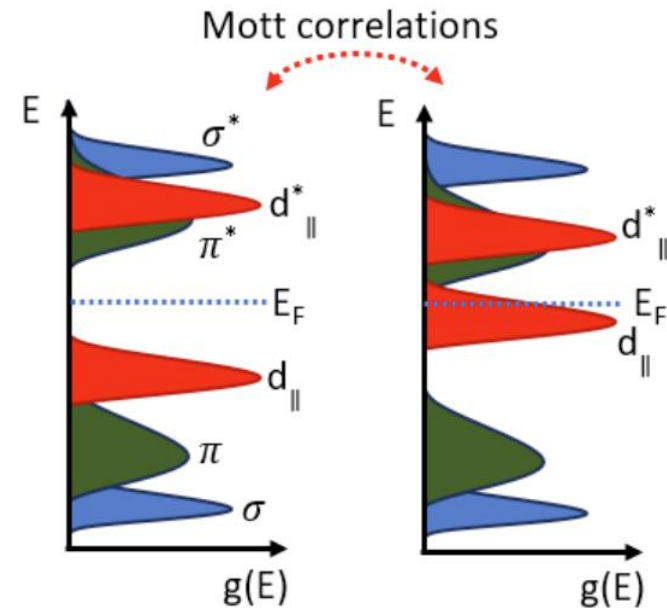
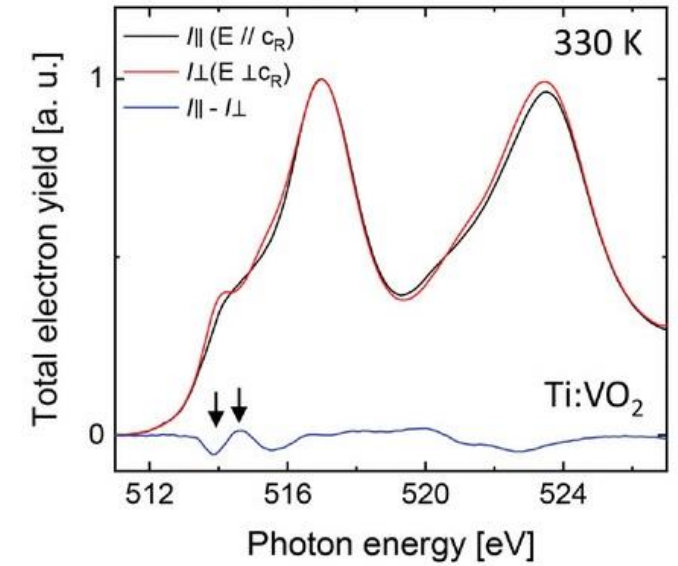
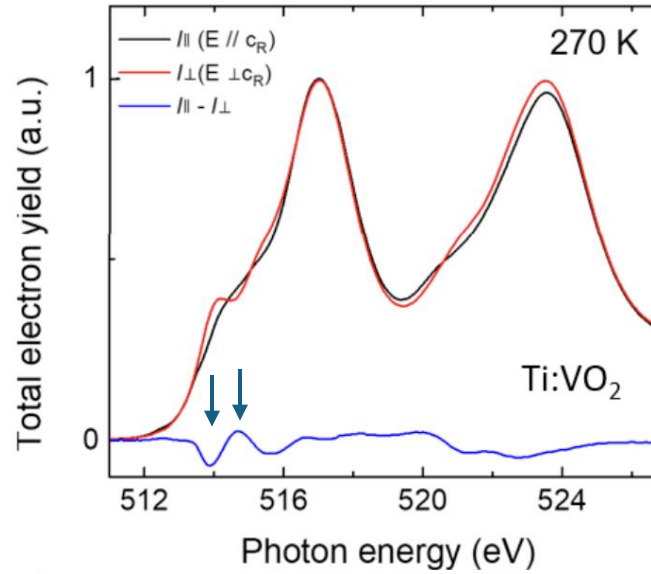
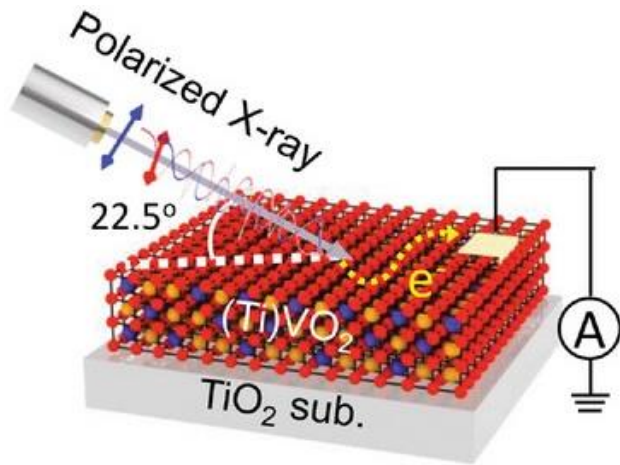
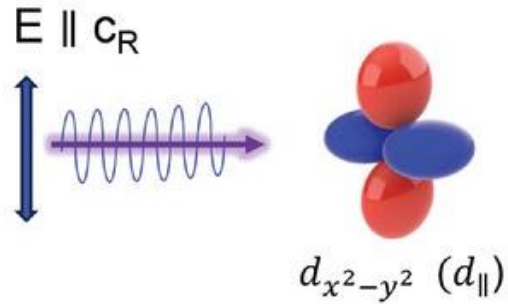
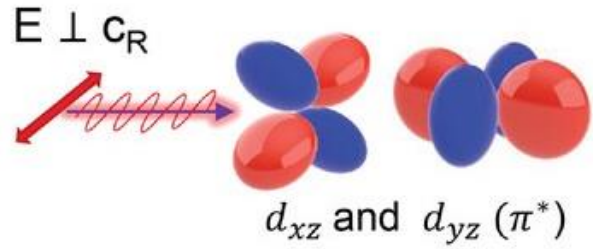
# Polarization-dependent XAS



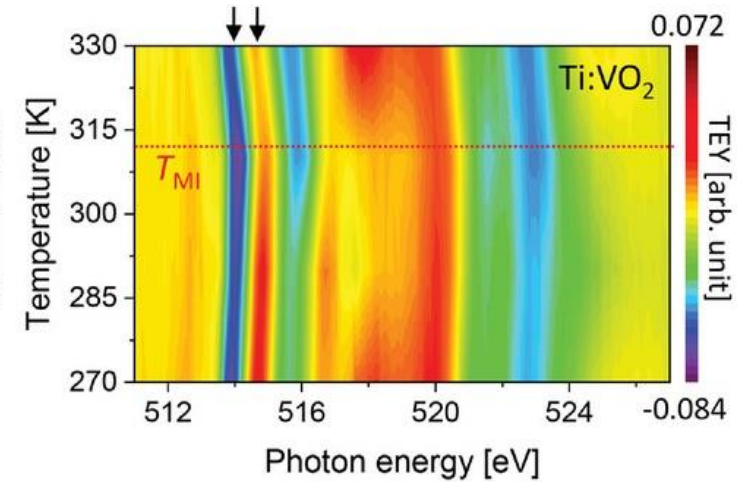
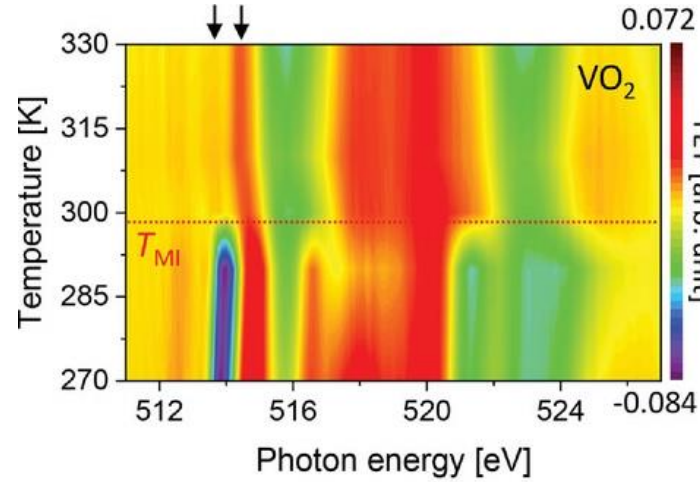
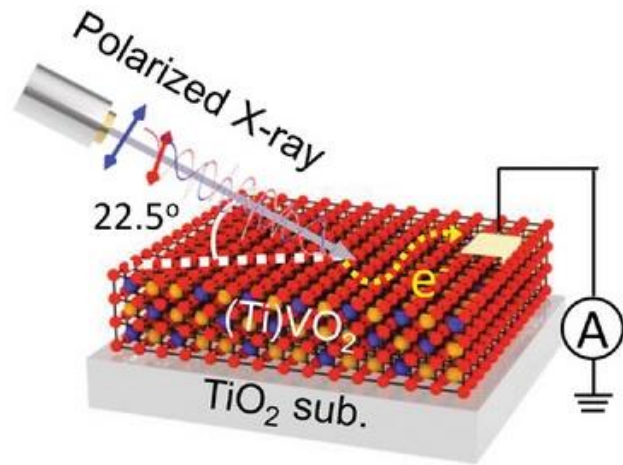
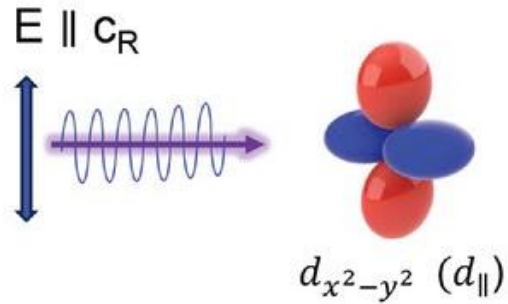
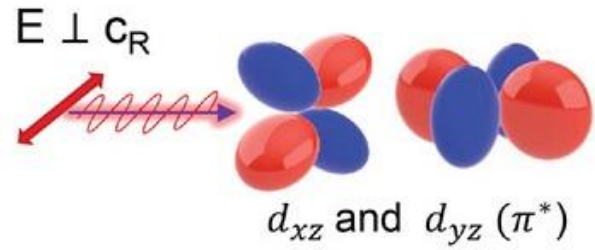
Peierls distortion + Mott correlations



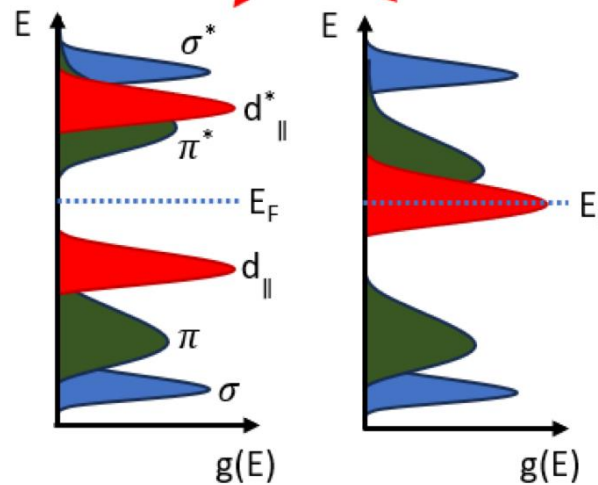
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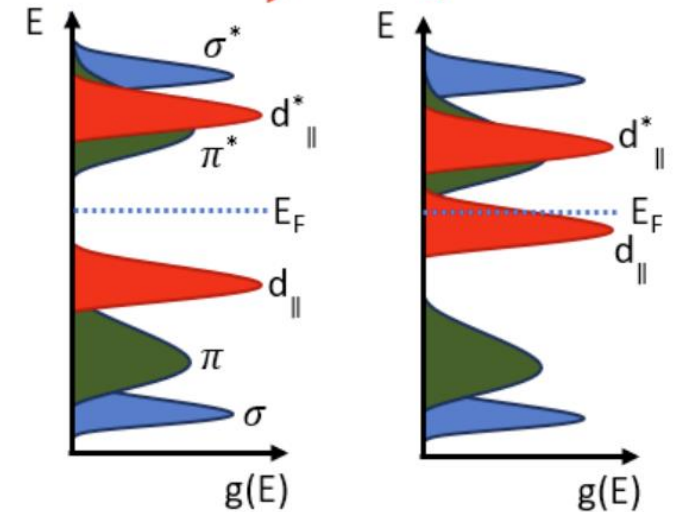
# Polarization-dependent XAS



Peierls distortion + Mott correlations

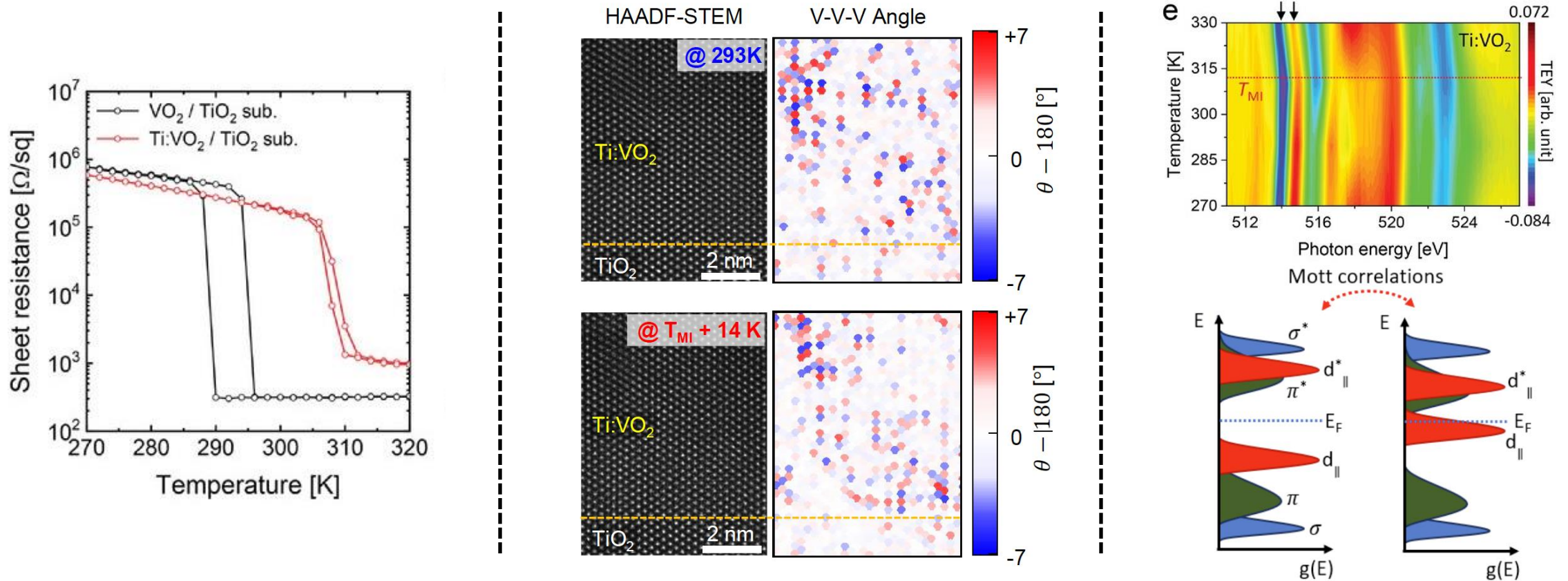


Mott correlations



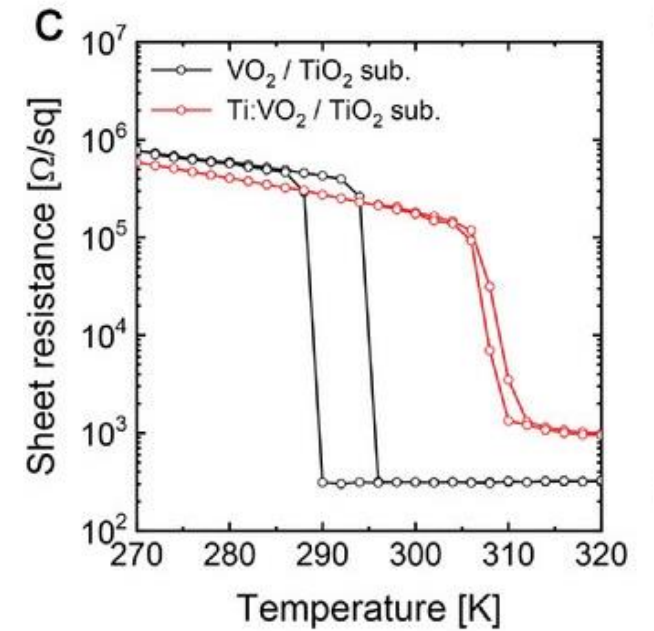
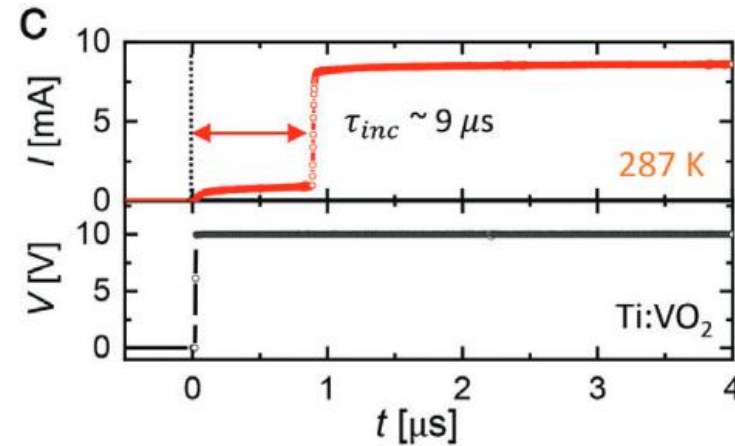
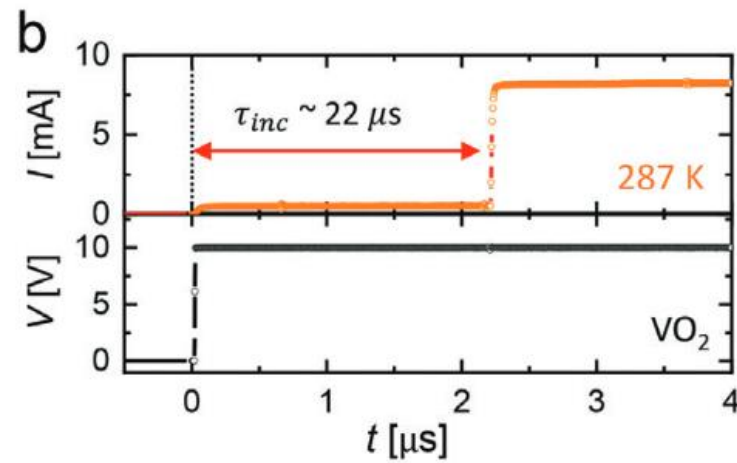
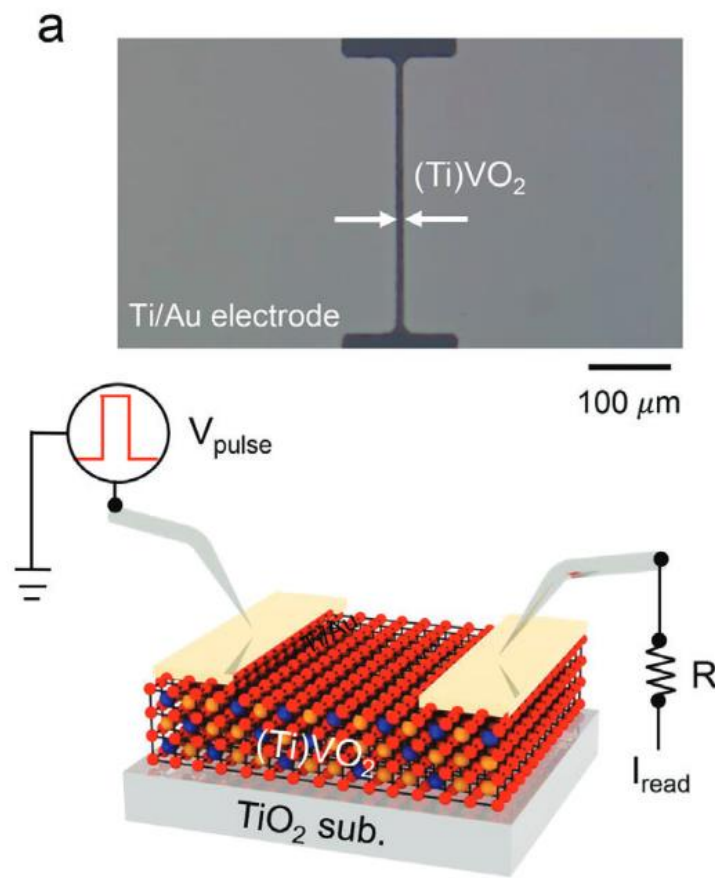
➤ localized V-V dimerization causes the persist orbital splitting above  $T_{MI}$ .

# Evidence of zero-strain metal insulator transition

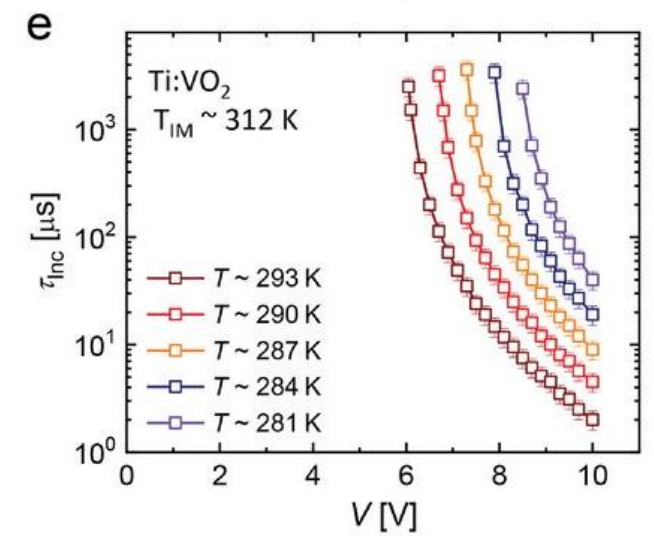
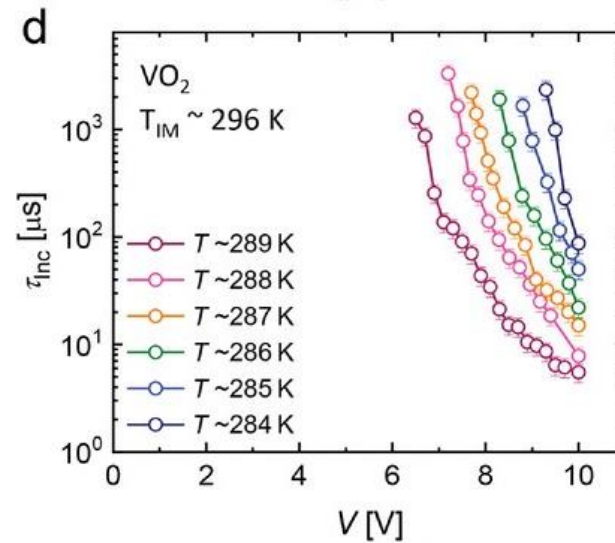
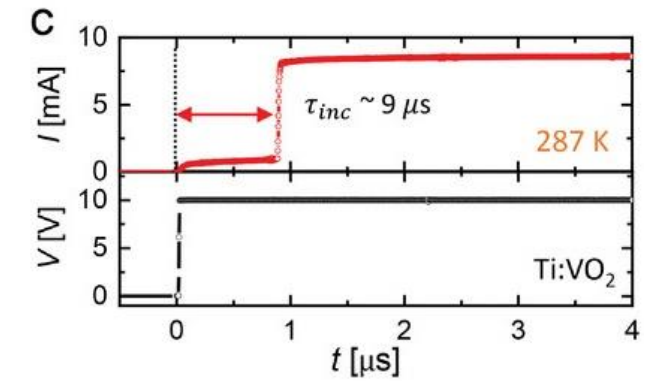
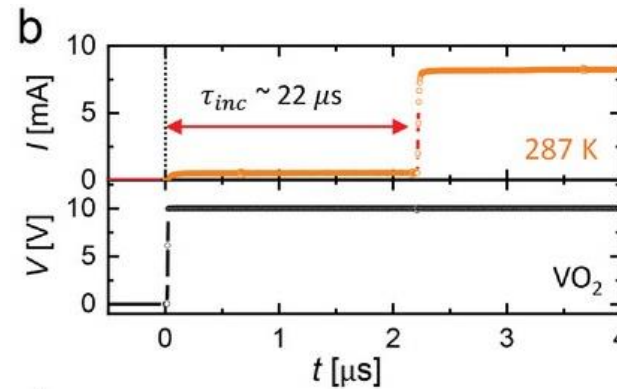
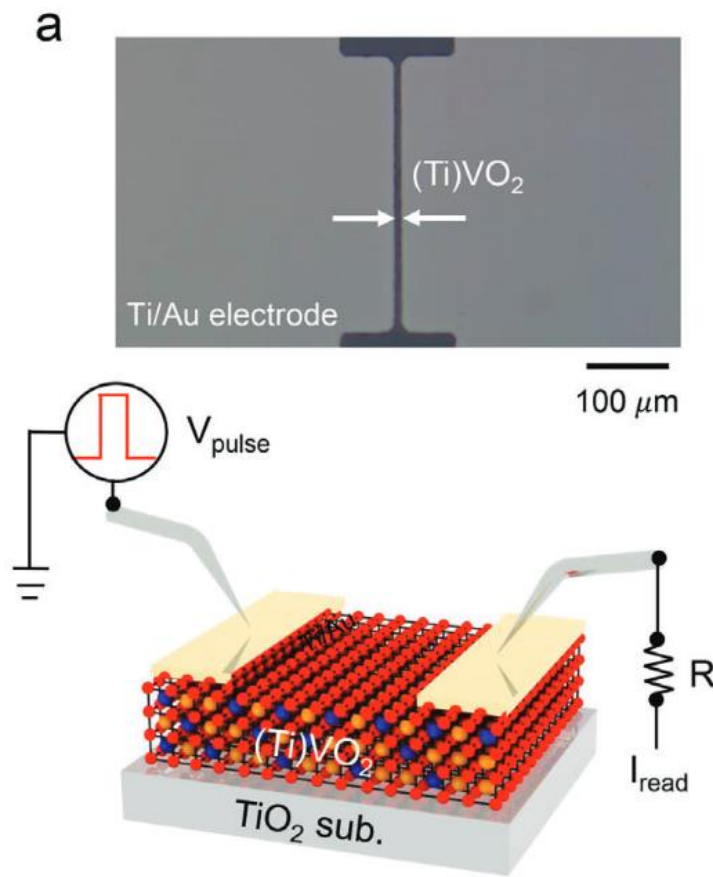


- Both measurements confirm that local atomic fluctuation by Ti incorporation results in zero-strain metal insulator transition.

# Switching dynamics using voltage pulses



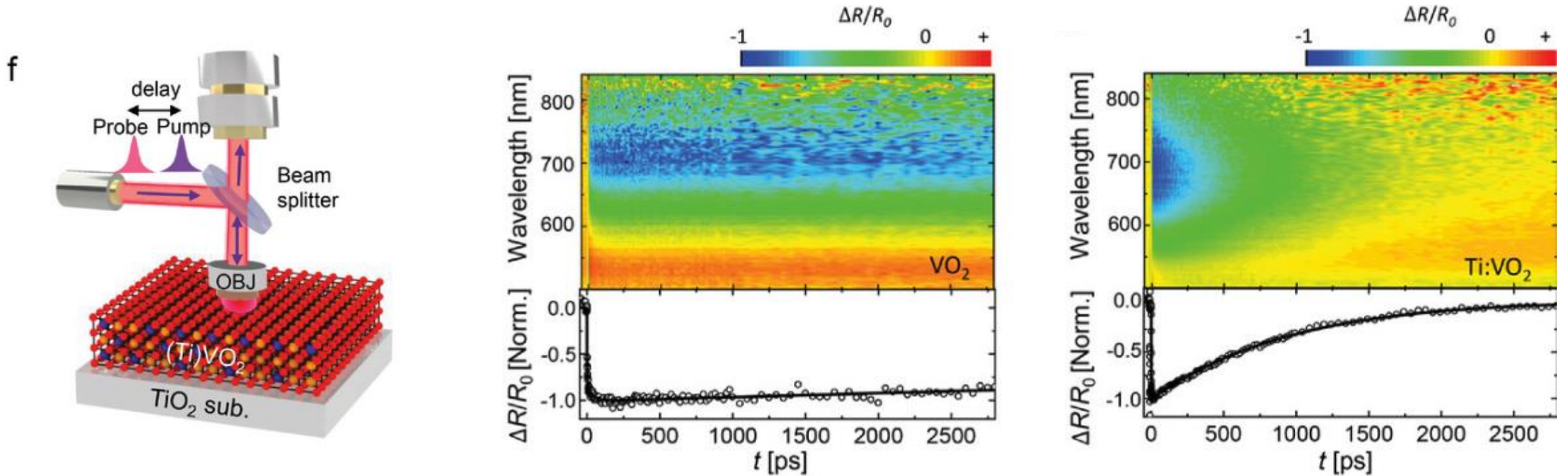
# Switching dynamics using voltage pulses



- Nanoscale structural heterogeneity enhances electrical switching dynamics due to geometrical compatibility at the interface.

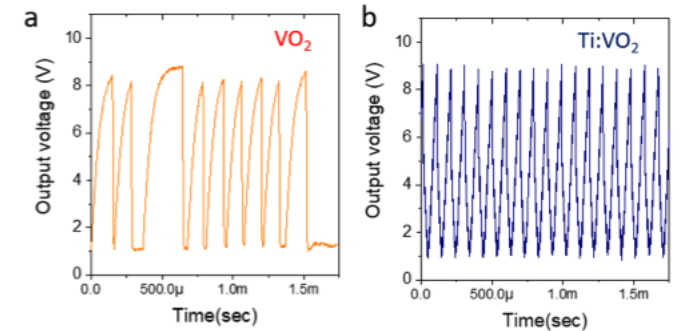
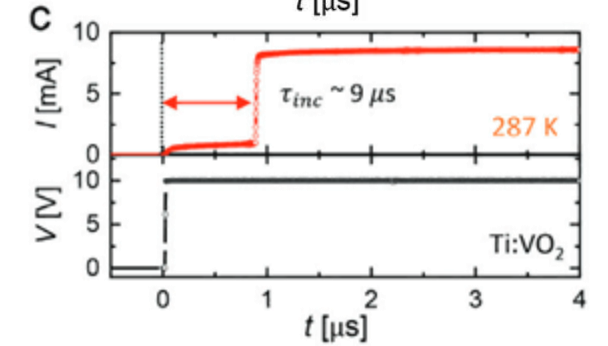
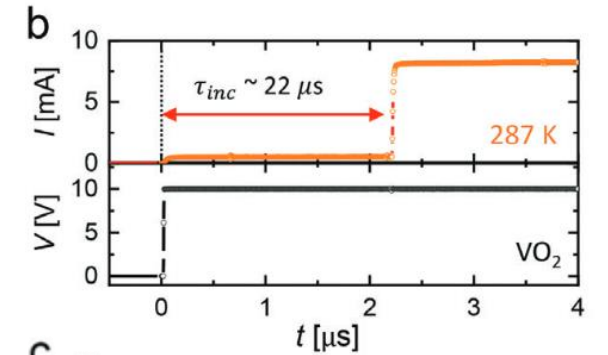
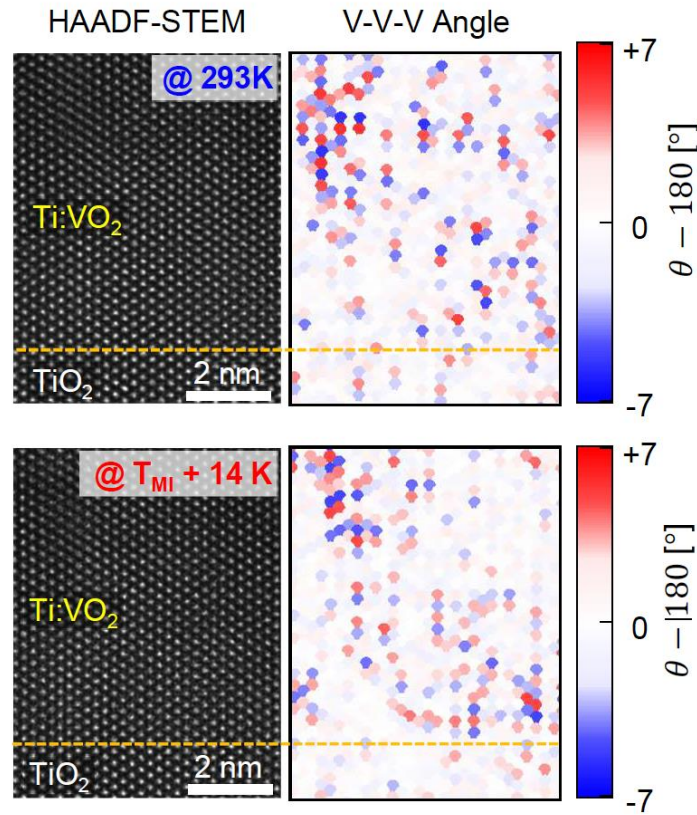
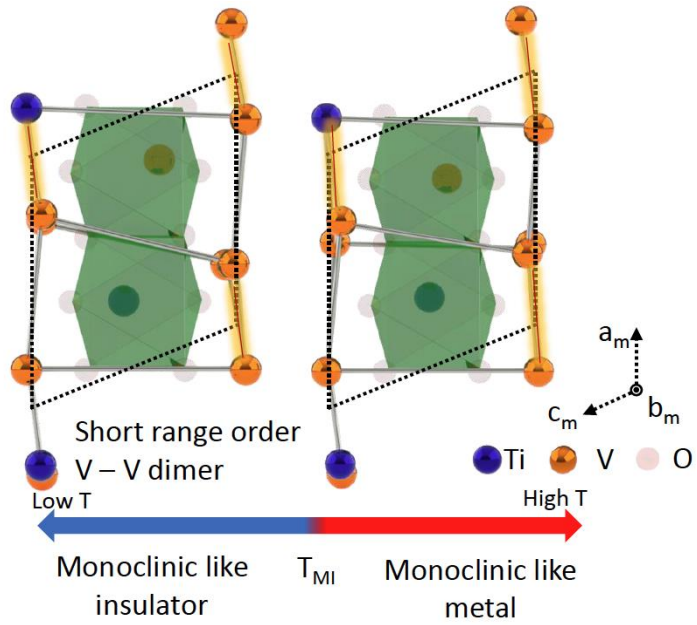
# Switching dynamics probed by THz spectroscopy

THz spectroscopy courtesy from Prof. O.-H. Kwon (UNIST)



- Compared with the slow recovery dynamics of undoped  $VO_2$ , the transient reflectivity of  $Ti:VO_2$  displays much faster relaxation.

# Summary 1



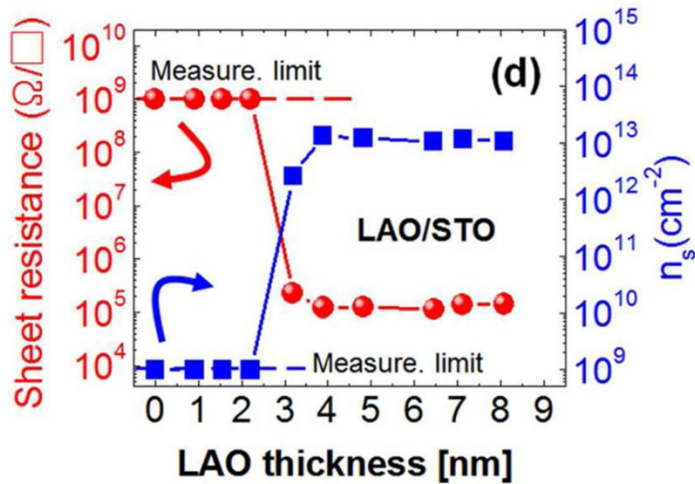
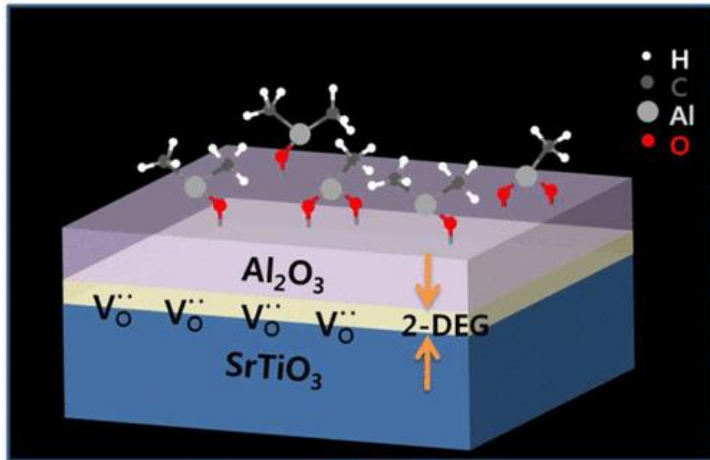
# Contents

## Topic 2 – 2D Vacancy Formation in Oxide Homo-interfaces for Enhanced Photocatalytic Activities



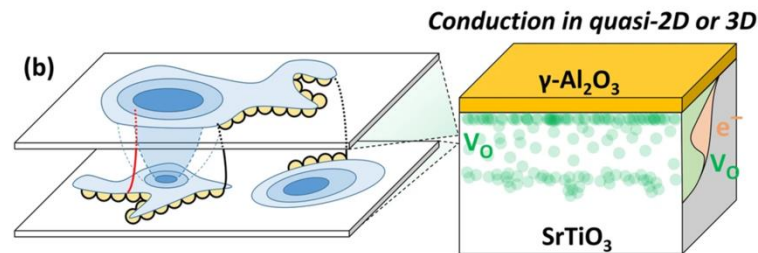
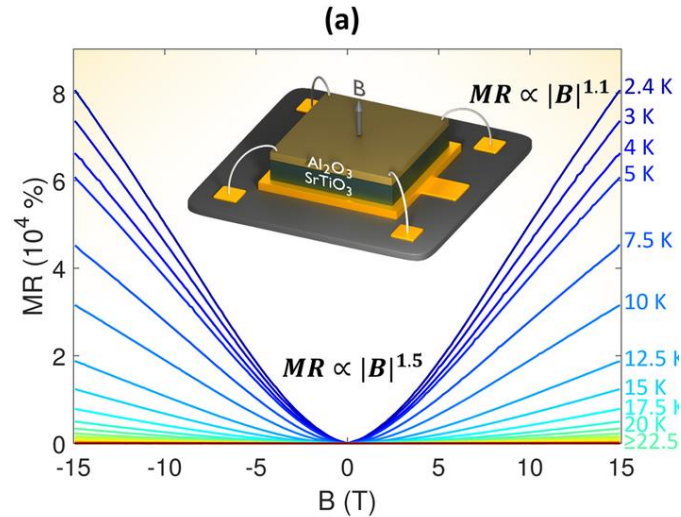
# The role of oxygen vacancies at hetero-interfaces

□ High mobility



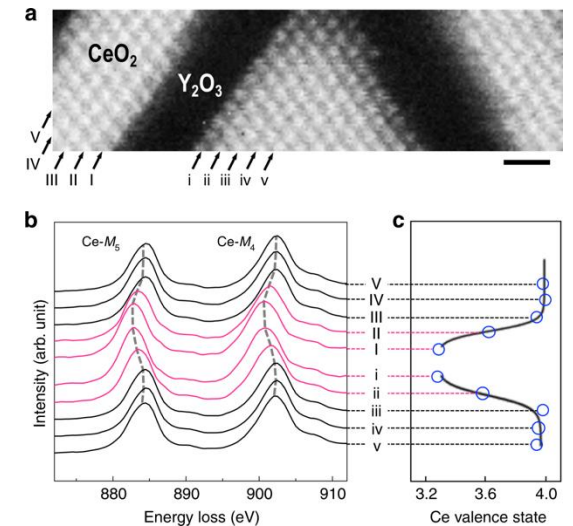
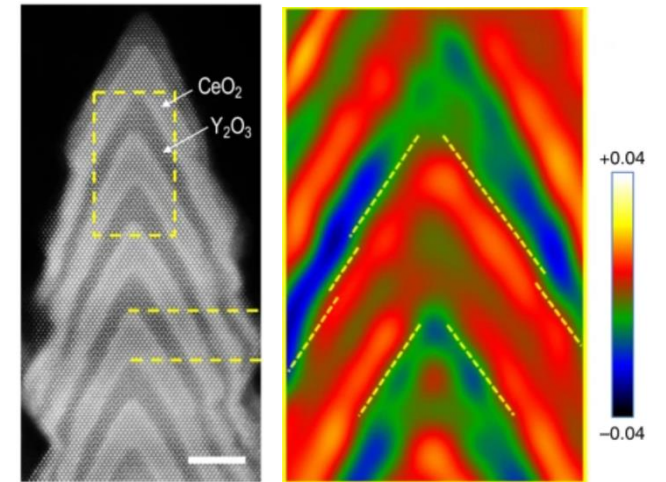
*Nano Lett.* **12**, 4775-4783 (2012)

□ XMR



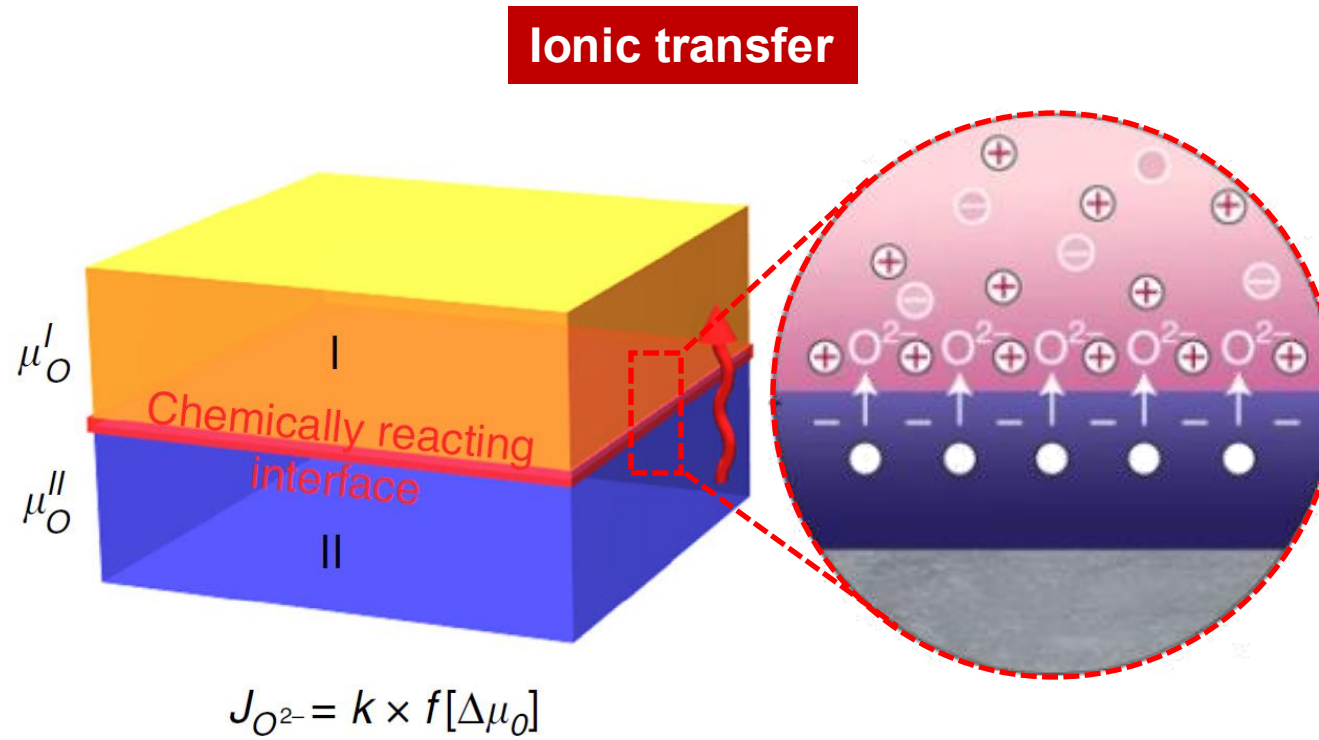
*Nat. Commun.* **15**, 4249 (2024)

□ Ionic conductor



*Nat. Commun.* **11**, 1371 (2020)

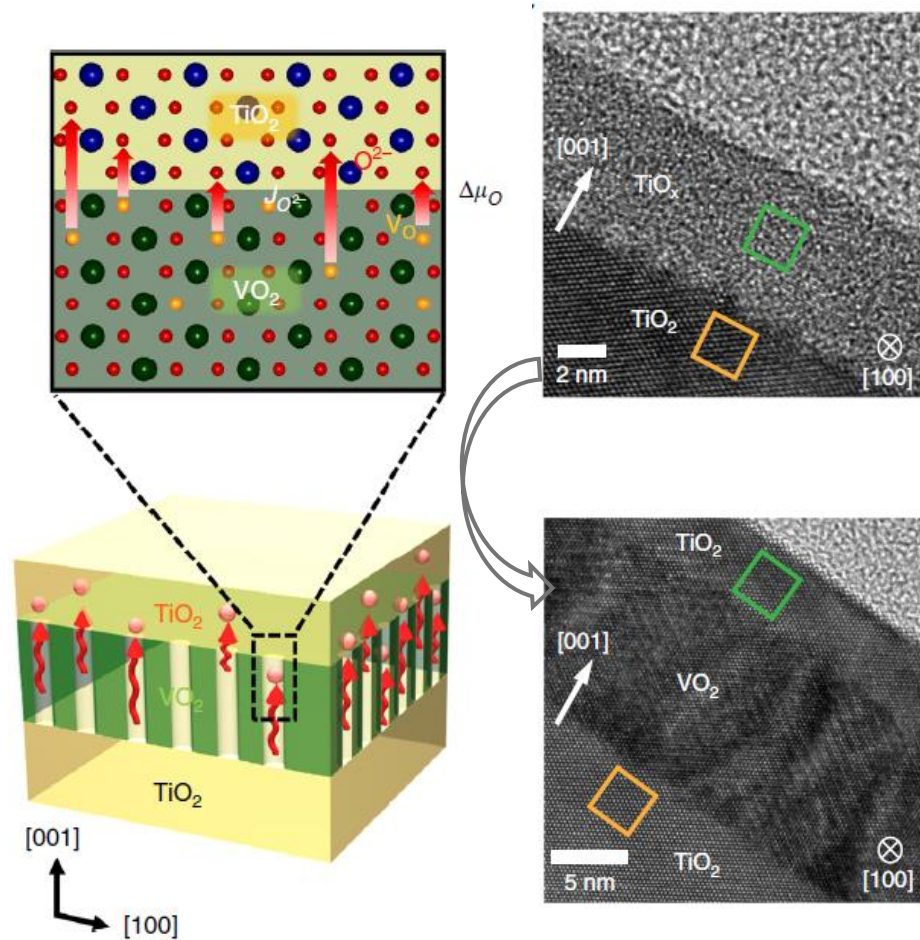
# Ionic transfer by heterogeneous interfaces



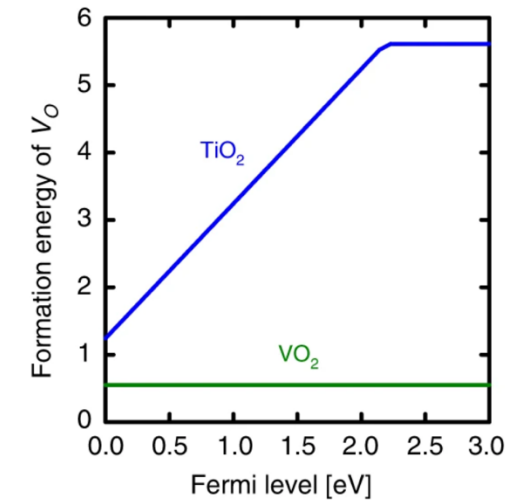
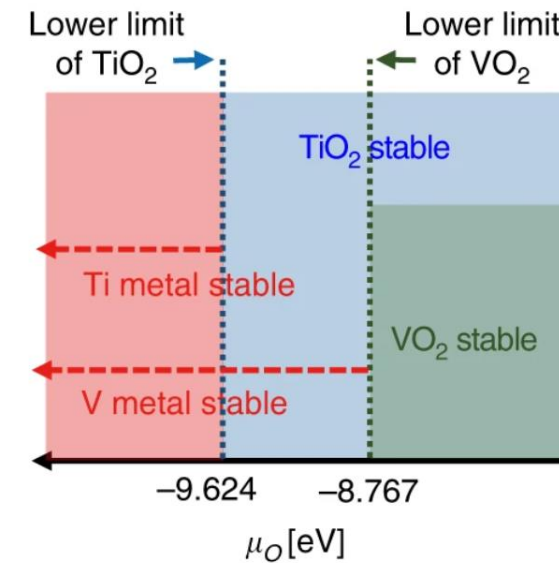
- Oxygen chemical potential mismatch between two different materials accelerates ionic migration.

# Directional oxygen transport for low-temp. epitaxy

## □ Low-temperature epitaxy



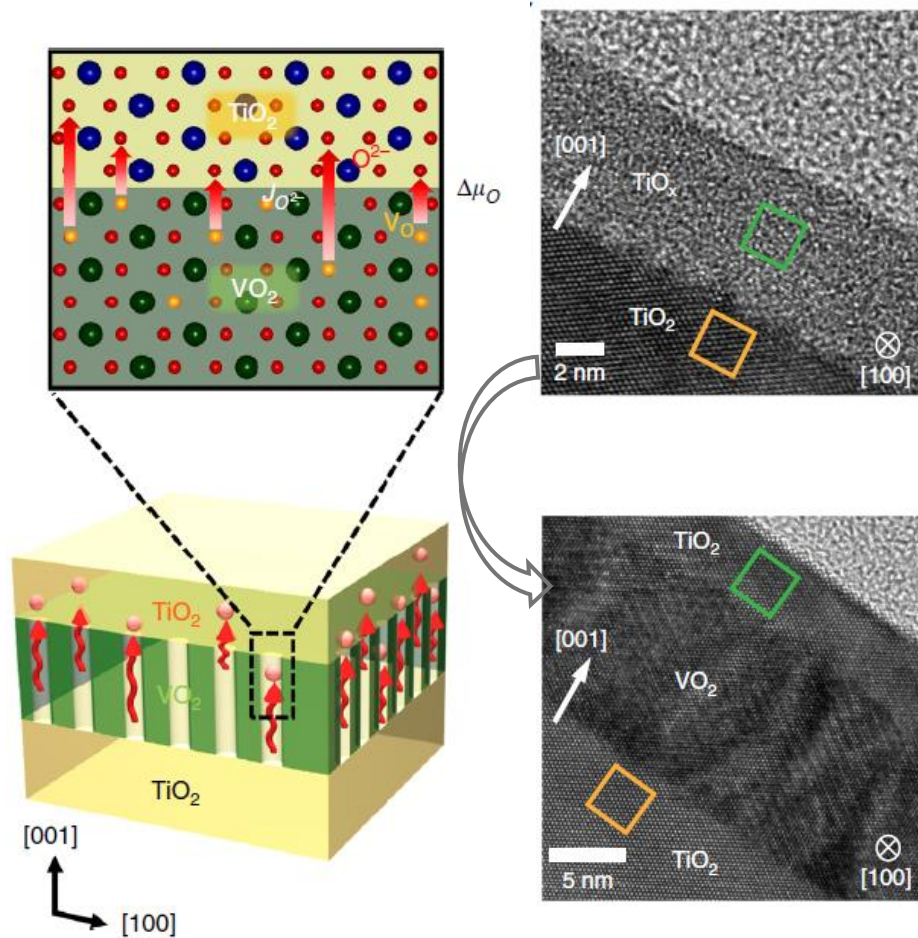
## 1) Oxygen chemical potential mismatch



DFT calculation courtesy from Prof. D. Lee (POSTECH)

# Directional oxygen transport for low-temp. epitaxy

## □ Low-temperature epitaxy



## 2) Chemical free energy change

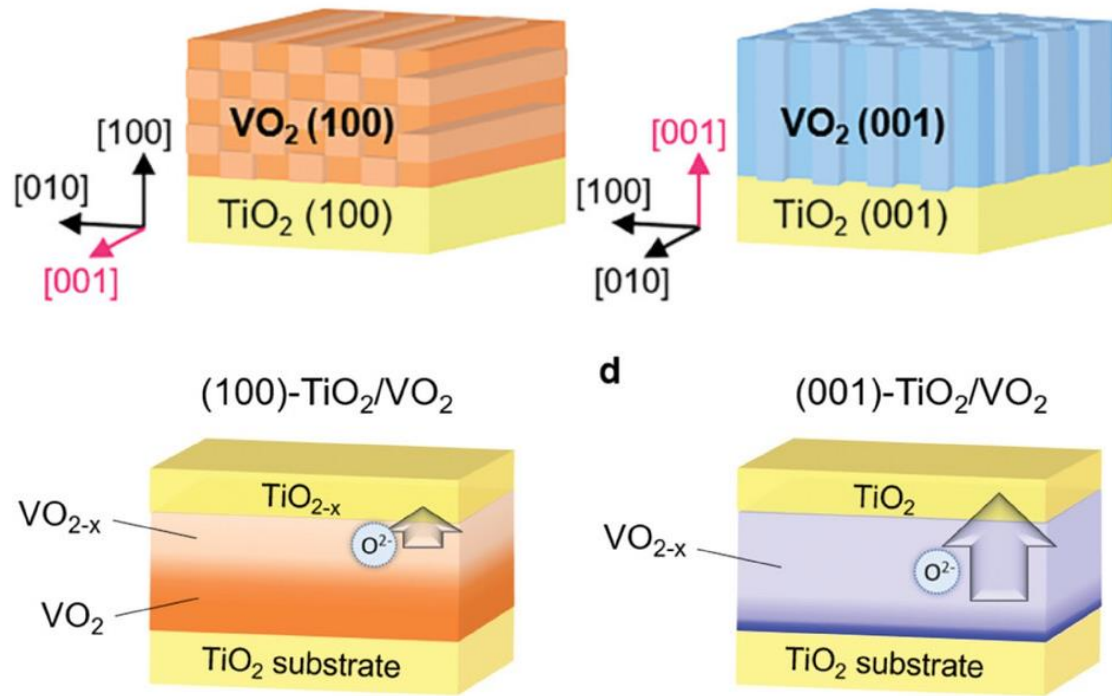
$$(2) \downarrow \Delta G^* = \frac{\overset{\text{surface free energy}}{16\pi\gamma_{fv}^3}}{\underset{\text{Chemical free energy change for formation of solid rutile TiO}_2}{3(\Delta G_v - \Delta G_s)^2}} \overset{\text{geometrical factor}}{S(\theta)} \uparrow (1)$$

Interfacial strain energy

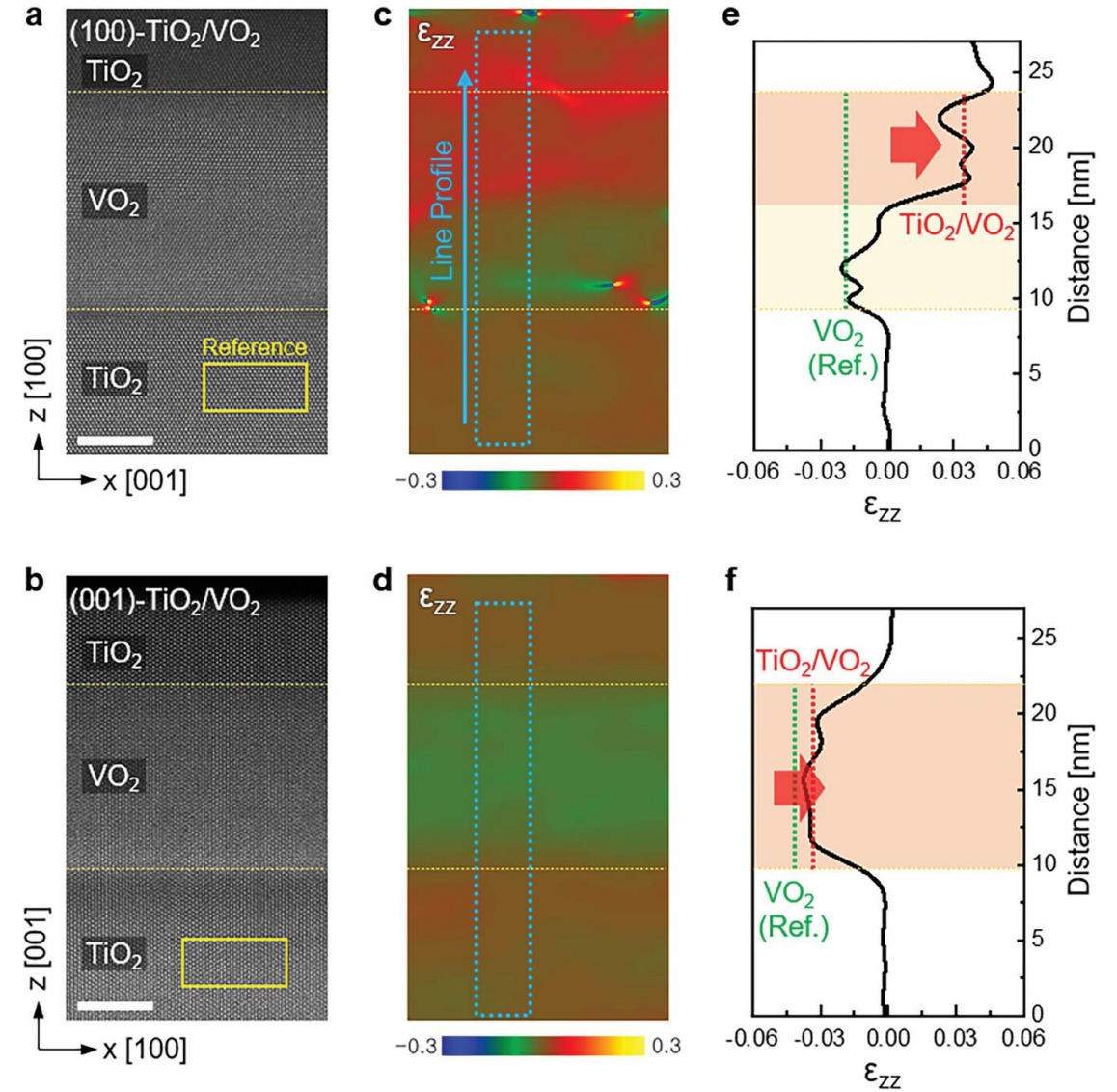
$$(4) \downarrow \frac{1}{\tau_{cryst}} = A \cdot \exp\left(-\frac{\Delta G^*}{k_B T_g}\right) \downarrow (3)$$

- ❖ Greater  $\Delta G_v$  induced by  $J_O$  significantly reduced  $\Delta G^*$  in hetero structure enables large reduction of  $\tau_{cryst}$  and unprecedented epitaxy.

# Crystallographic pathway-dependent ionic transport



Small. 20, 2402260 (2024)

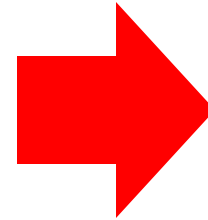


# Formation of interfacial $V_O$ in arbitrary thin films

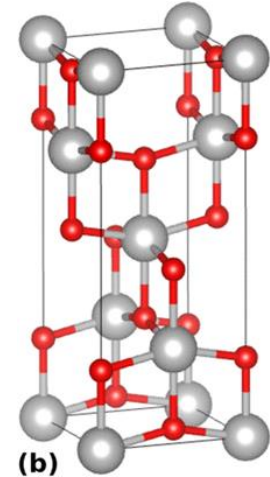
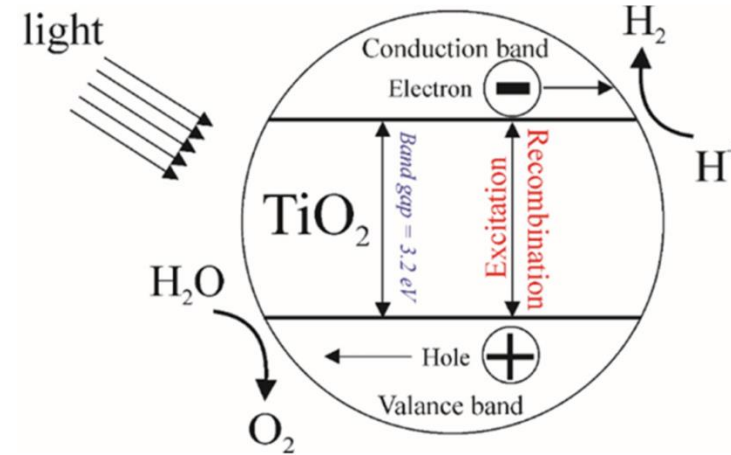
1) Oxygen chemical potential mismatch

2) Chemical free energy change

3) Crystallographic orientation



## □ TiO<sub>2</sub>-based photocatalyst

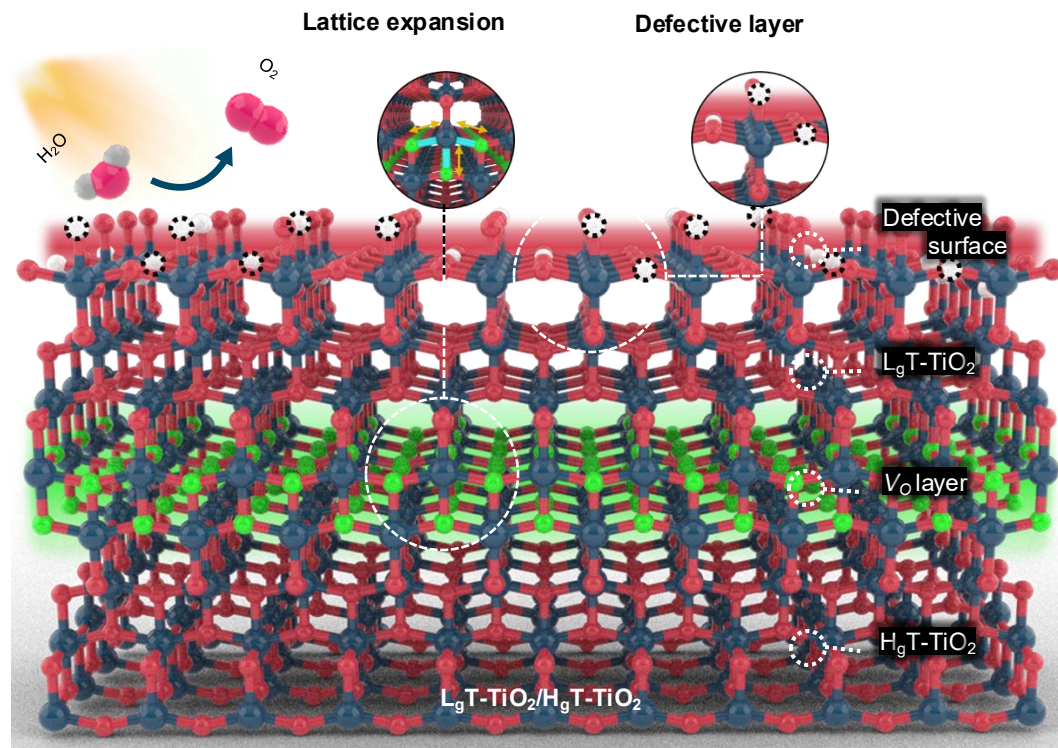


*Nanomaterials* **10**, 1790 (2020)

*Chemical Review* **114**, 9919-9986 (2014)

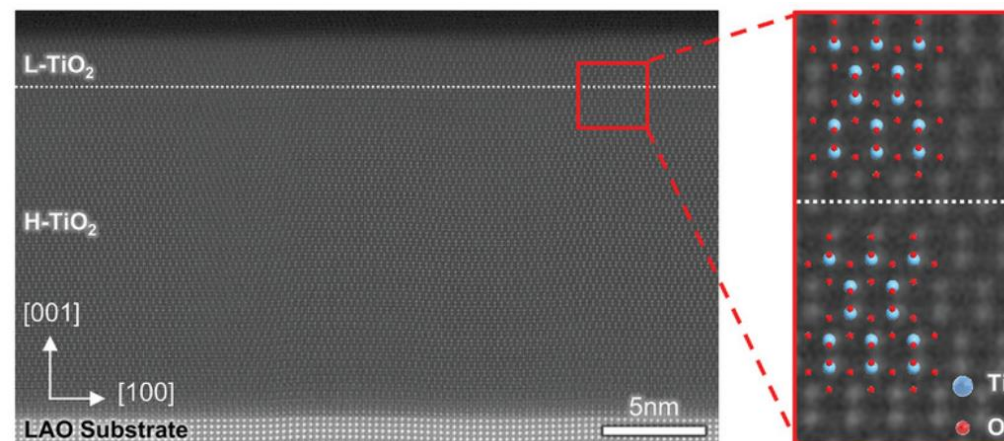
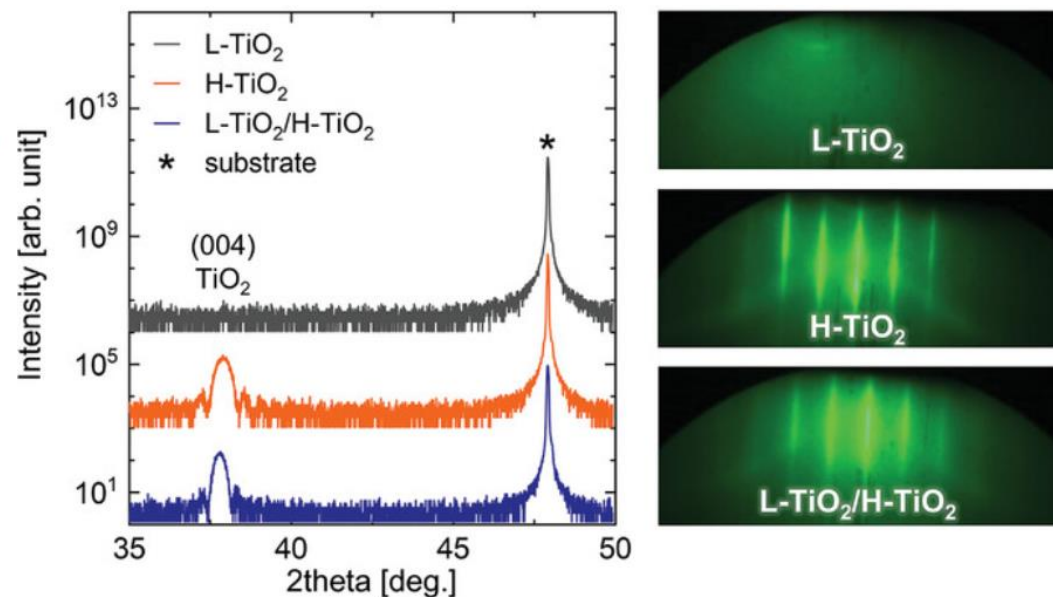
- suitable band gap
- high stability
- non-toxic and environmentally friendly
- Abundance and low cost

# Synthesis of TiO<sub>2</sub> homo structure



*Adv. Mater.* 2413062 (2025)

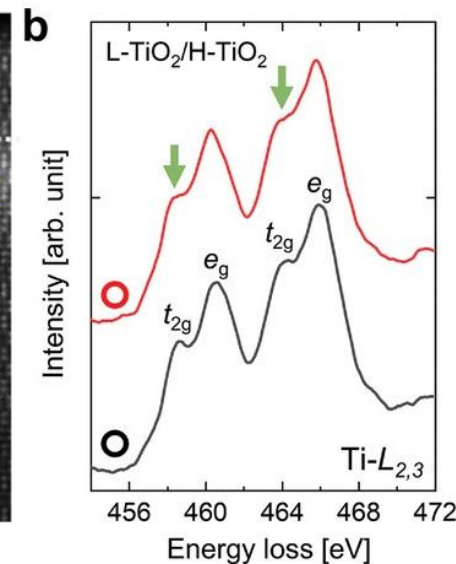
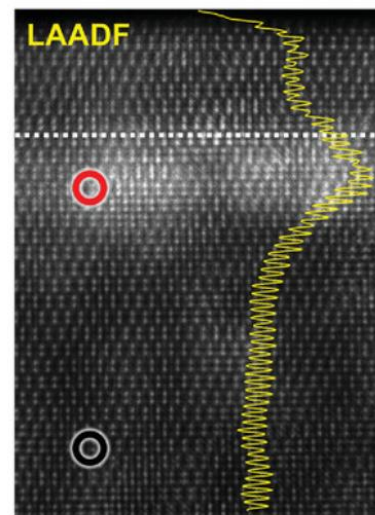
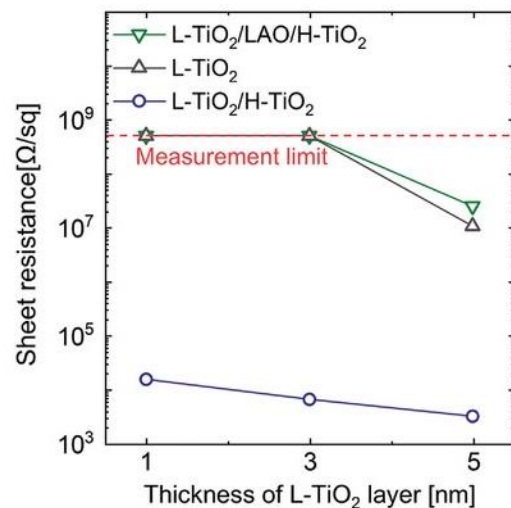
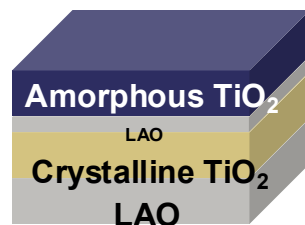
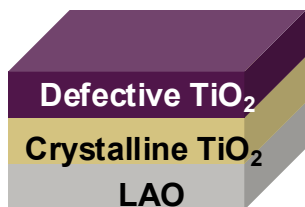
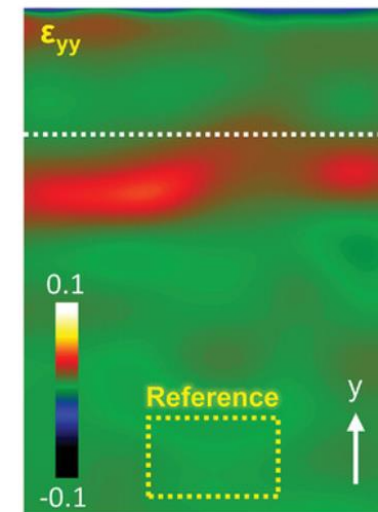
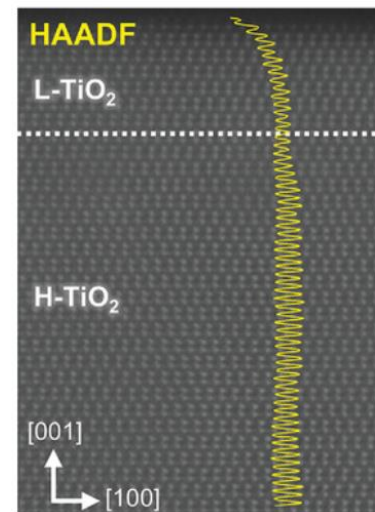
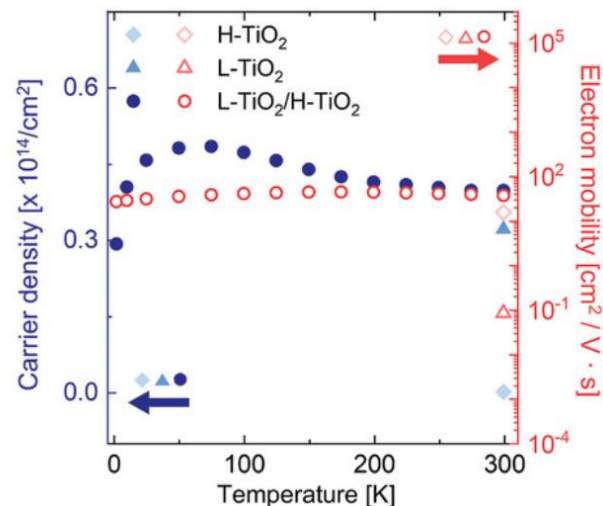
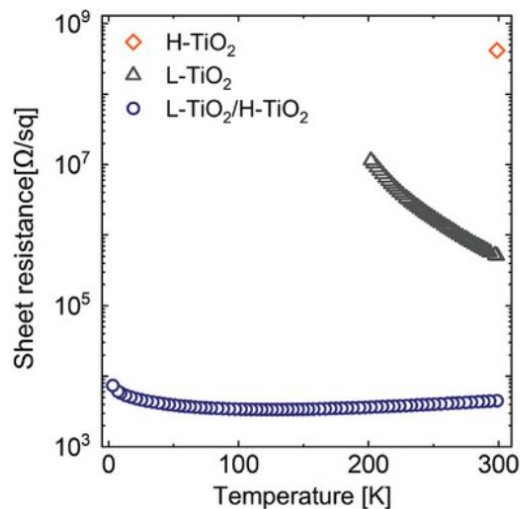
STEM images courtesy from Prof. S.-Y. Choi (POSTECH)



*Adv. Mater.* 37, 2413062 (2025)

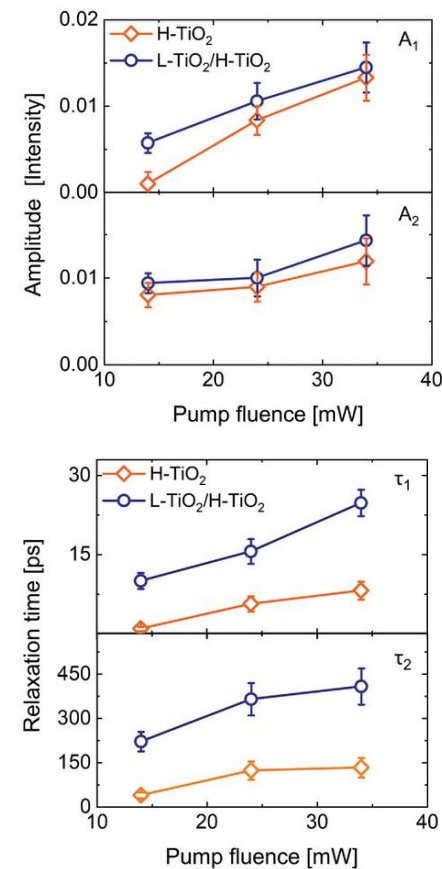
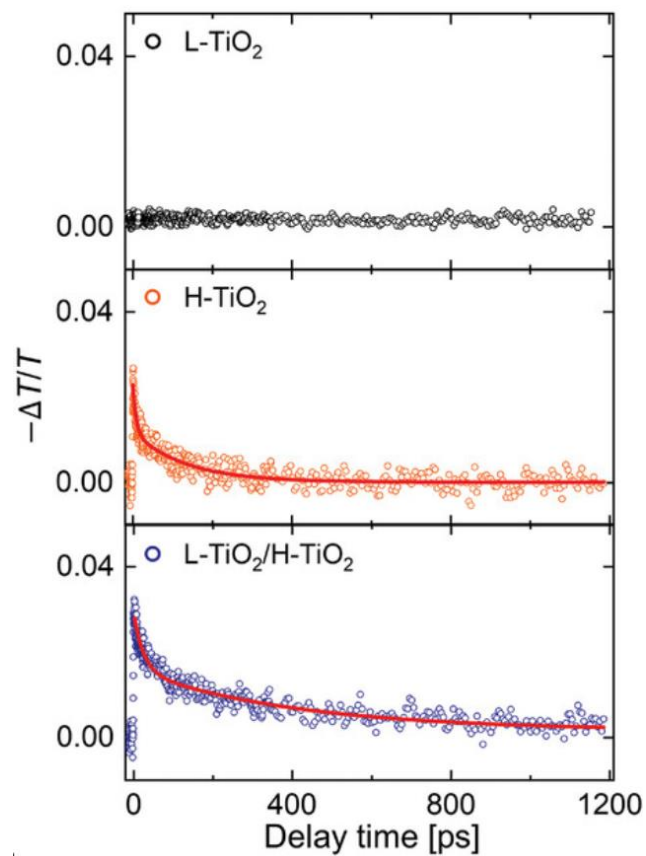
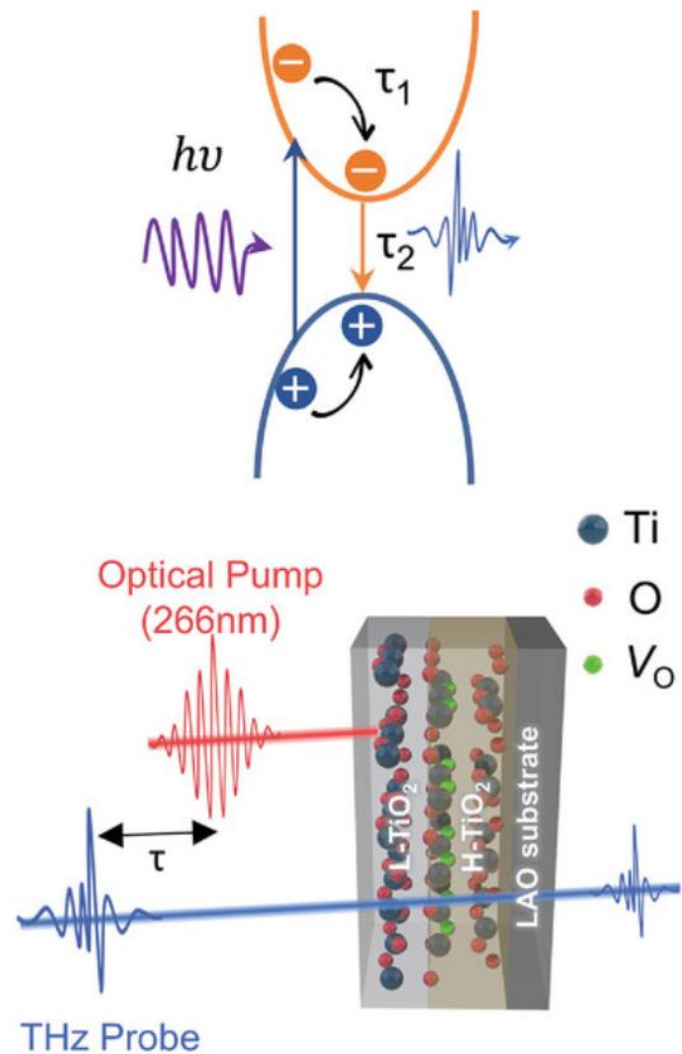
# Revealing interfacial oxygen vacancies

STEM images courtesy from Prof. S.-Y. Choi (POSTECH)



Adv. Mater. 37, 2413062 (2025)

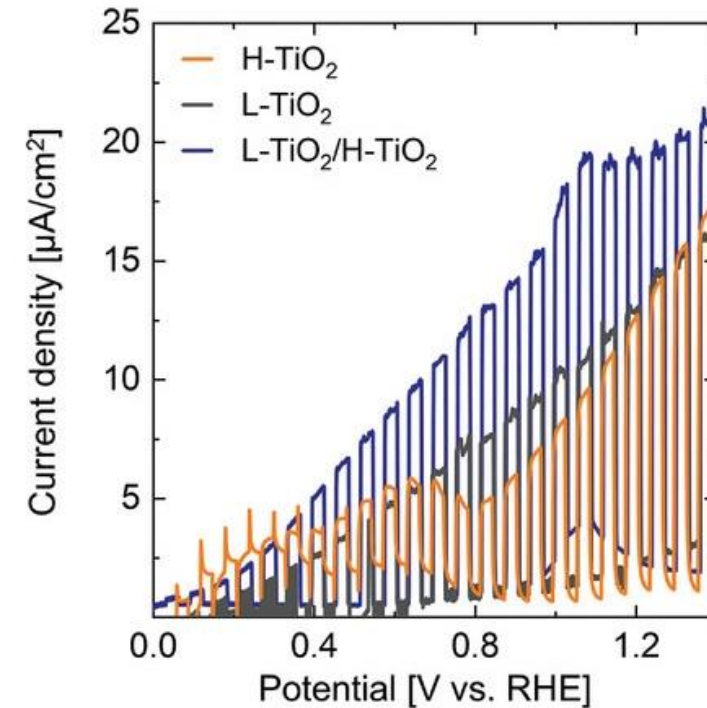
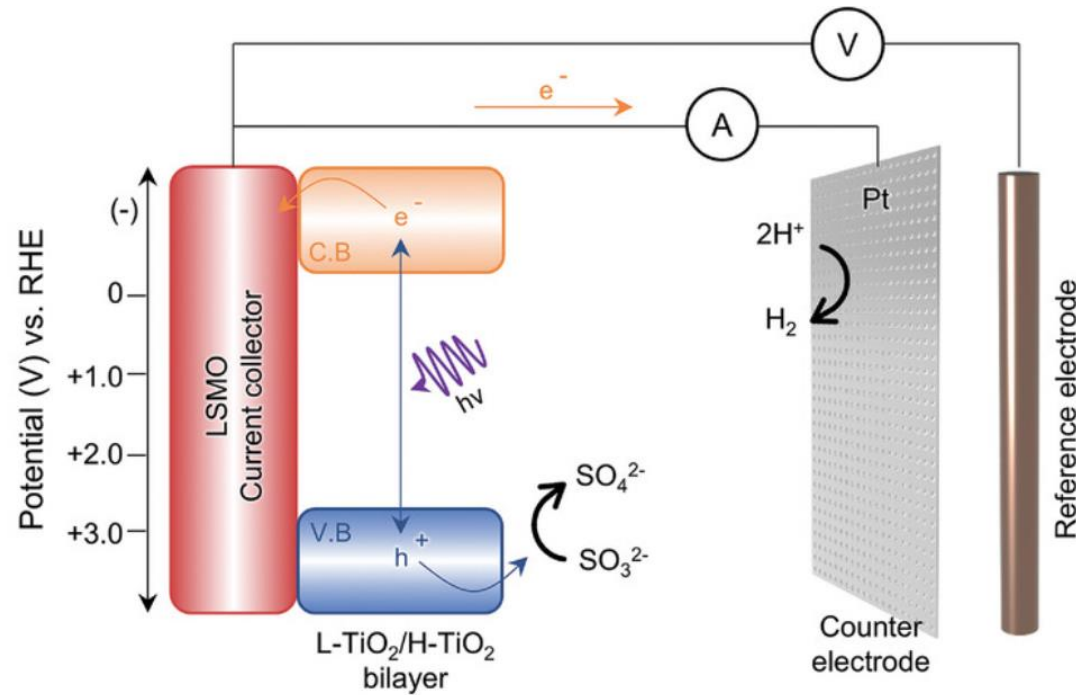
# Long-lived photocarrier dynamics



$$-\frac{\Delta T}{T}(t) = \left(-\frac{\Delta T}{T}\right)_0 + A_1 e^{-\frac{t}{\tau_1}} + A_2 e^{-\frac{t}{\tau_2}}$$

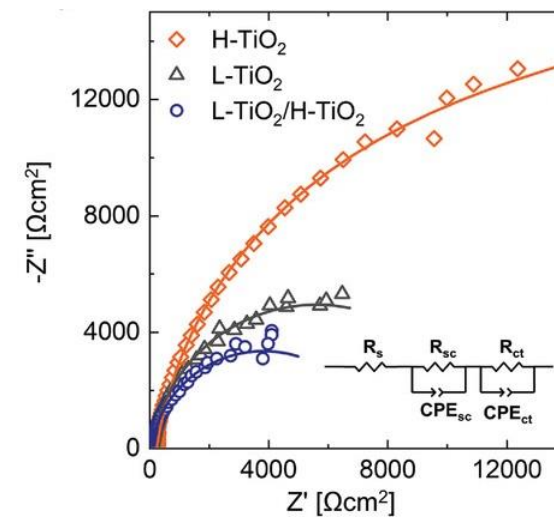
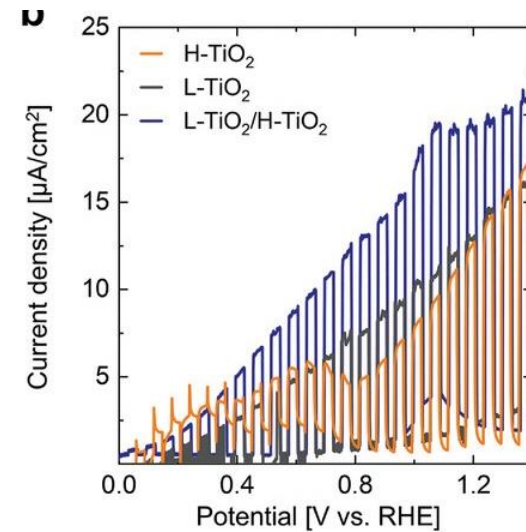
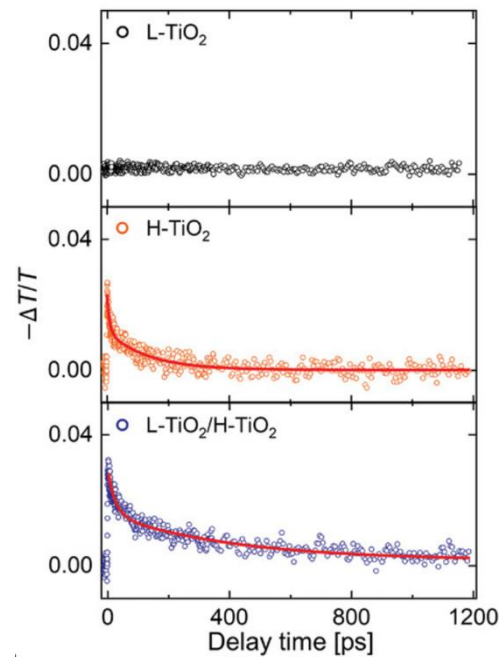
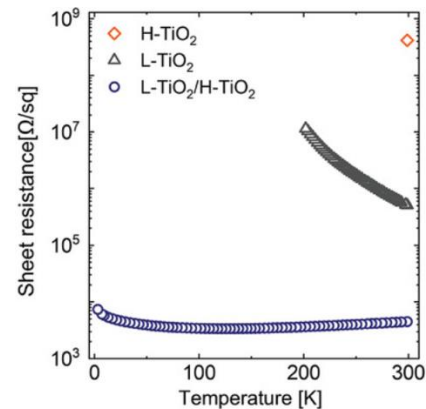
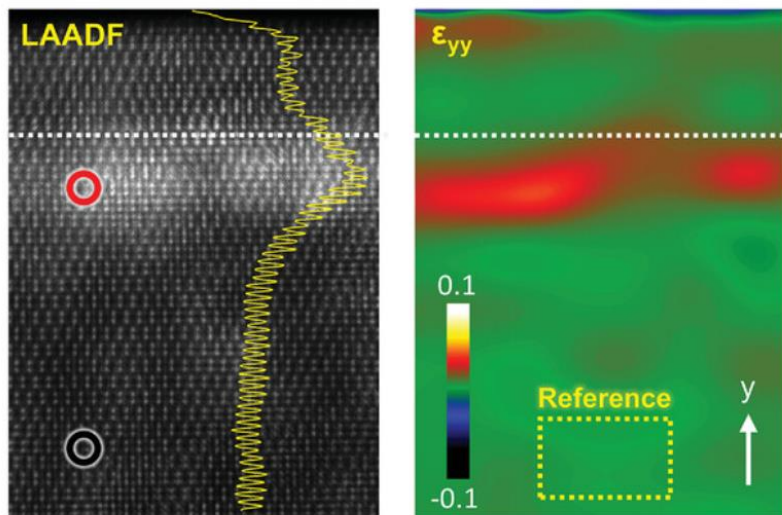
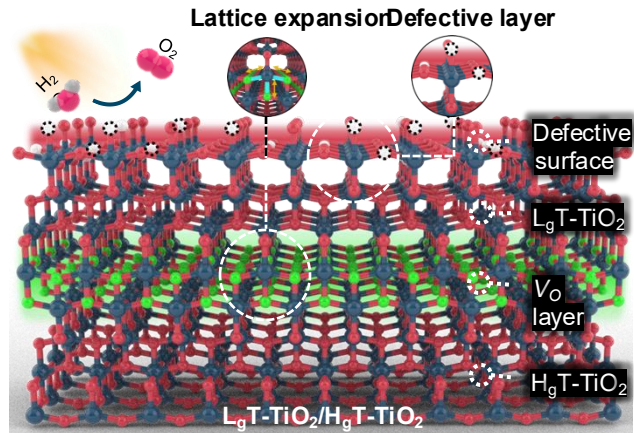
# Promotion of PEC activities

PEC measurement courtesy from Prof. H. W. Jang (SNU)



- The conductive interface with high carrier density in the L-TiO<sub>2</sub>/H-TiO<sub>2</sub> bilayer accelerates the electron transfer process to generate a photocatalytic reaction.

# Summary 2



# Acknowledgement



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Prof. Donghwa Lee



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