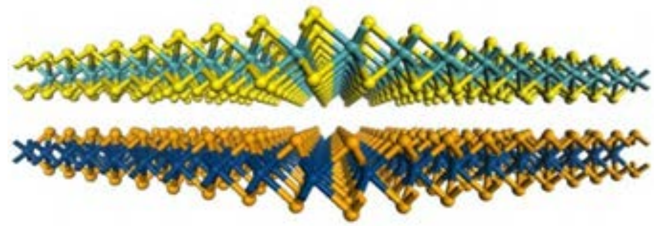
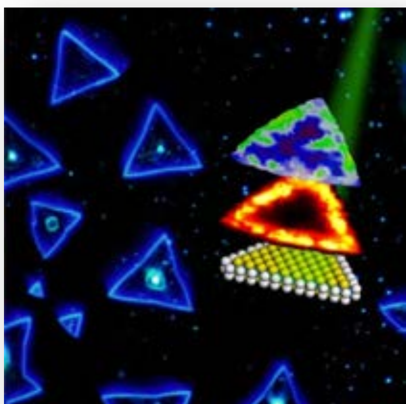
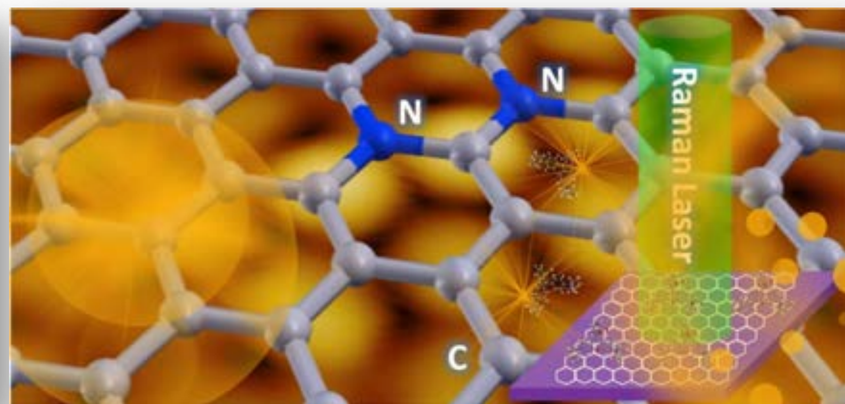
Center for 2-Dimensional and Layered Materials Penn State



Defect Engineering in 2D Materials: Doped Graphene and Beyond

Mauricio Terrones





Department of Physics, Chemistry & Materials Science and Engineering, Center for 2-Dimensional and Layered Materials, The Pennsylvania State University, USA and Institute of Carbon Science and Technology, Shinshu University, JAPAN

Center for 2-Dimensional and Layered Materials Penn State

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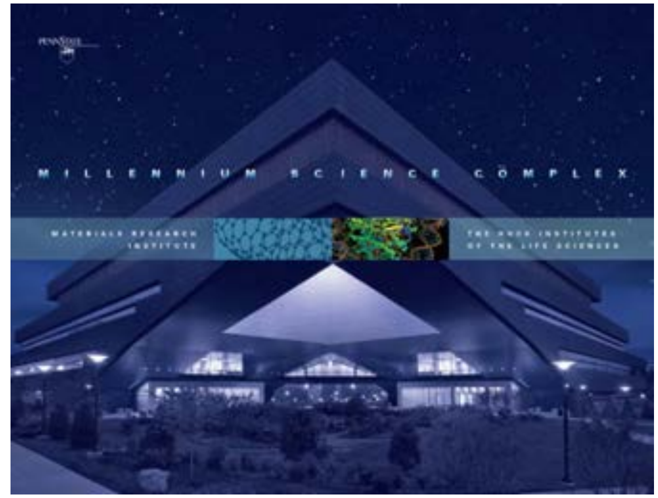
SHINSHU UNIVERSITY

Center for 2-Dimensional and Layered Materials
Penn State

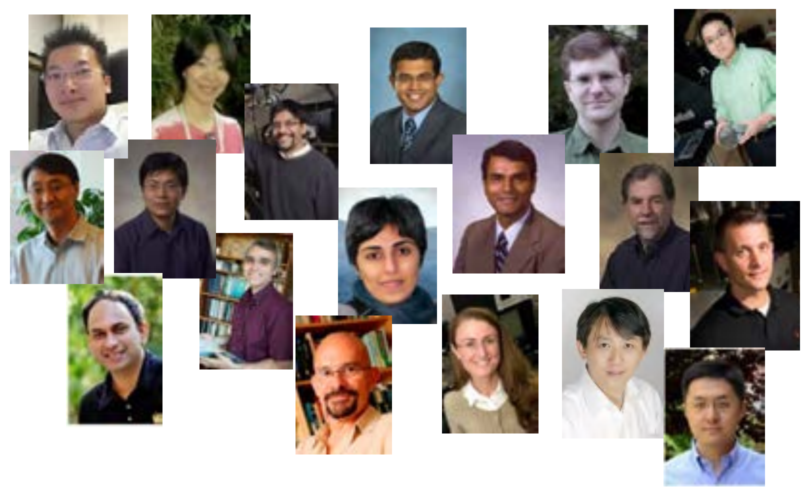


Director

Mauricio Terrones

Assoc. Director

Joshua Robinson



http://www.mri.psu.edu/centers/2dlm/

Center for 2-Dimensional and Layered Materials Penn State

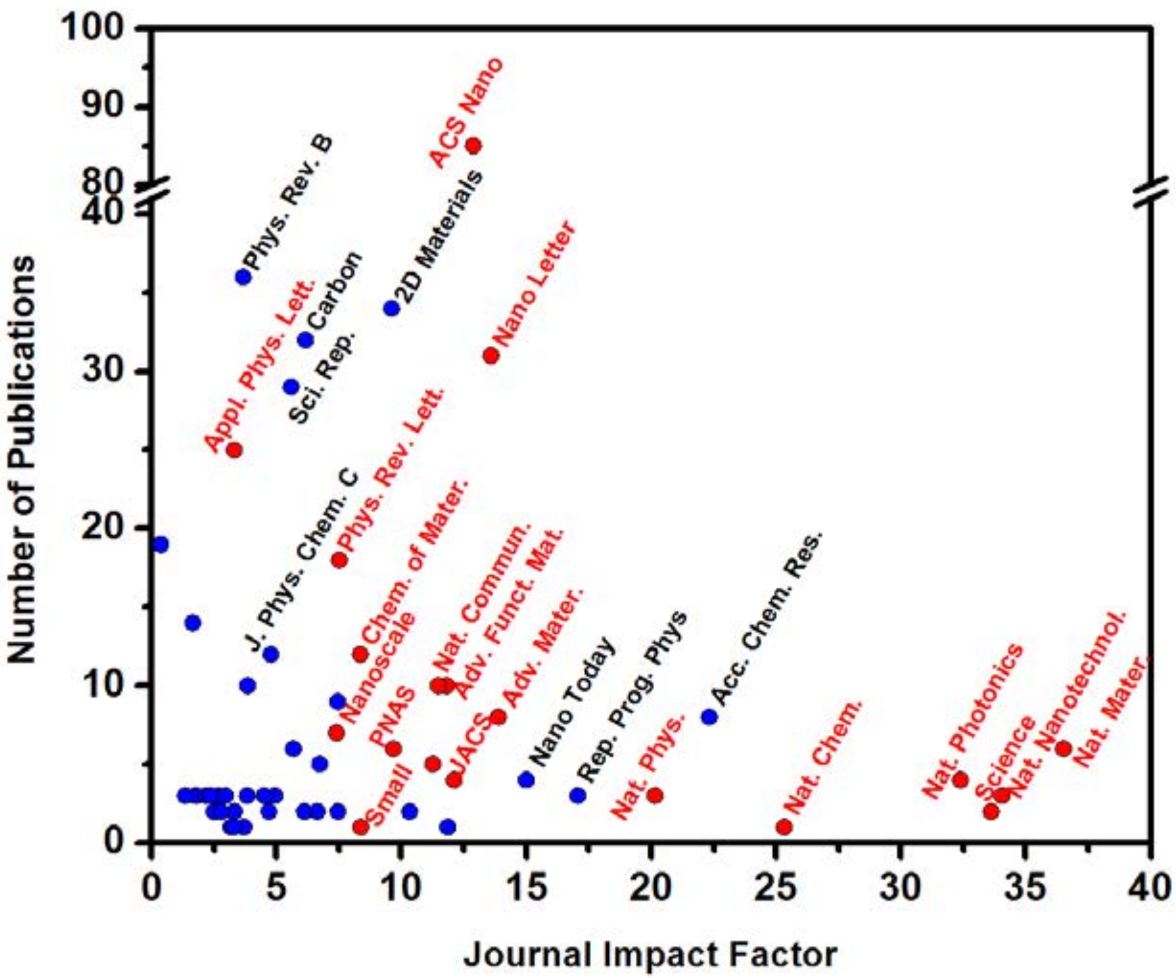
Multidisciplinary 2D Research Center at Penn State

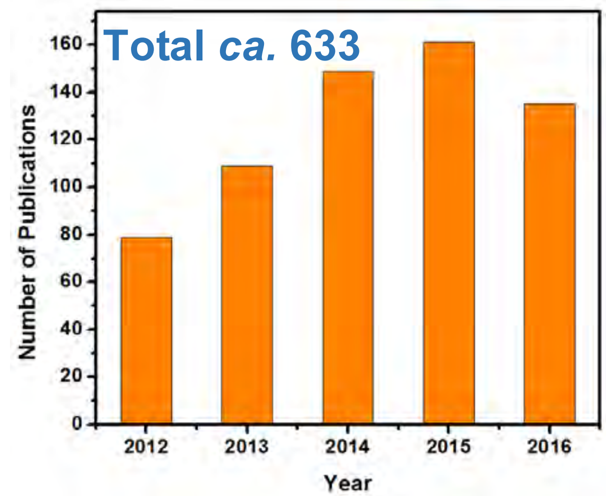
Faculty	
Nasim Alem	Tom Mallouk
Moses Chan	Suzanne Mohney
Vincent Crespi	Joan Redwing
Sukwon Choi	Joshua Robinson
Ismaila Dabo	Nitin Samarth
Saptarshi Das	Ray Schaak
Aman Haque	Jie Shan
Eric Hudson	Susan Sinnot
R. Engel-Herbert	Jorge Sofo
Tom Jackson	Mauricio Terrones
Seong H. Kim	Adri van Duin
Ying Liu	Douglas Wolfe
Zhiwen Liu	Sulin Zhang
Kin Fai Mak	Jun Zhu

Research Associates/Post-Docs/Students	
Michael Abraham	Minh An Nguyen
Amin Azizi	Lavish Pabbi
Zakaria Al Balushi	Nestor Perea
Ganesh Rahul Bhimanapati	Lakshmy Pulickal Rajukumar
Abraham Cano	Chris Rotella
Donna D. Deng	Dr Eduardo Cruz Silva
Anna Domask	Ivan Skachko
Haila Al Dosari	Yifan Sun
Sarah Eichfeld	Youjian Tang
Dr. Ana Laura Elias	Timothy Walter
Simin Feng	Junjie Wang
Robert Douglas Fraleigh	Yuanxi Wang
Jarod Gagnon	Zefang Wang
Yiyang Gong	Xiaoxiang Xi
Corey T. Janisch	Kehao Zhang
Ethan Kahn	Xiaotian Zhang
Nina Kovtyukhova	Liang Zhao
Chia-Hui (Candace) Lee	Rui Zhao
Yu-Chuan Lin	Chanjing Zhou
Zhong Lin	
Debangshu Mukherjee	

We are... >30 Faculty and >40 Students/Post-docs Strong.

Articles Published at Penn State in 2D





CENTER FOR 2-DIMENSIONAL AND LAYERED MATERIALS

Two New NSF-Funded Research Centers

ATOMIC

Center for Atomically Thin Multifunctional Coatings

Academic Research in Partnership with and Guided by Industry

PENNSTATE

RICE

Director

Mauricio Terrones

Co-Director

Joshua Robinson

Co-Director

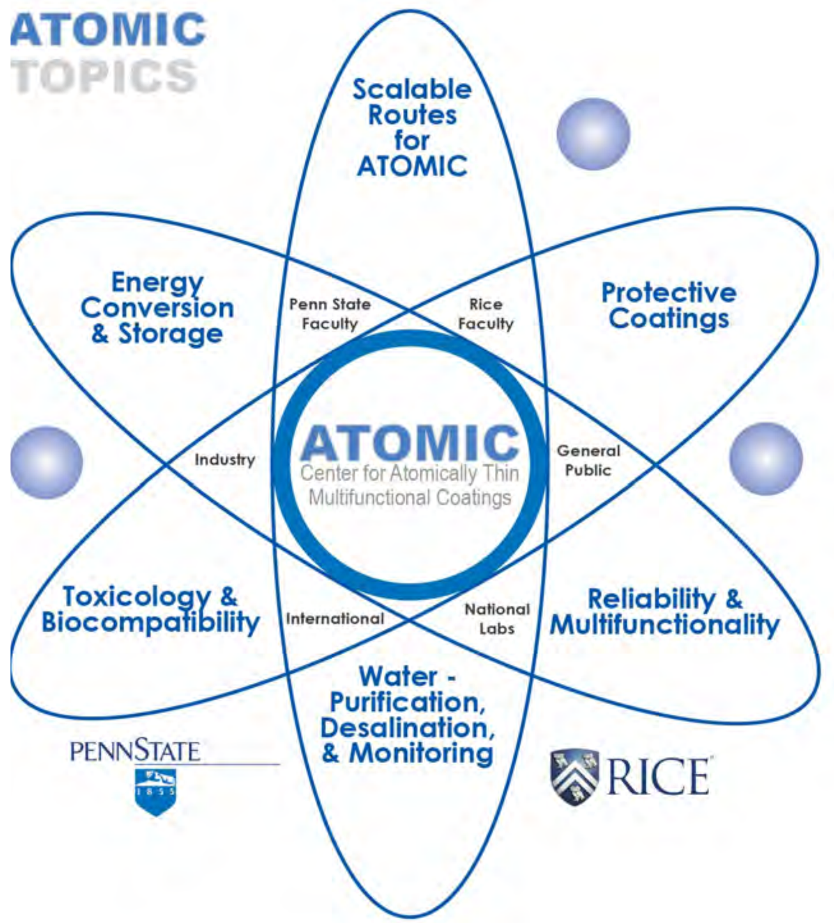
Pulickel Ajayan

Site. Director

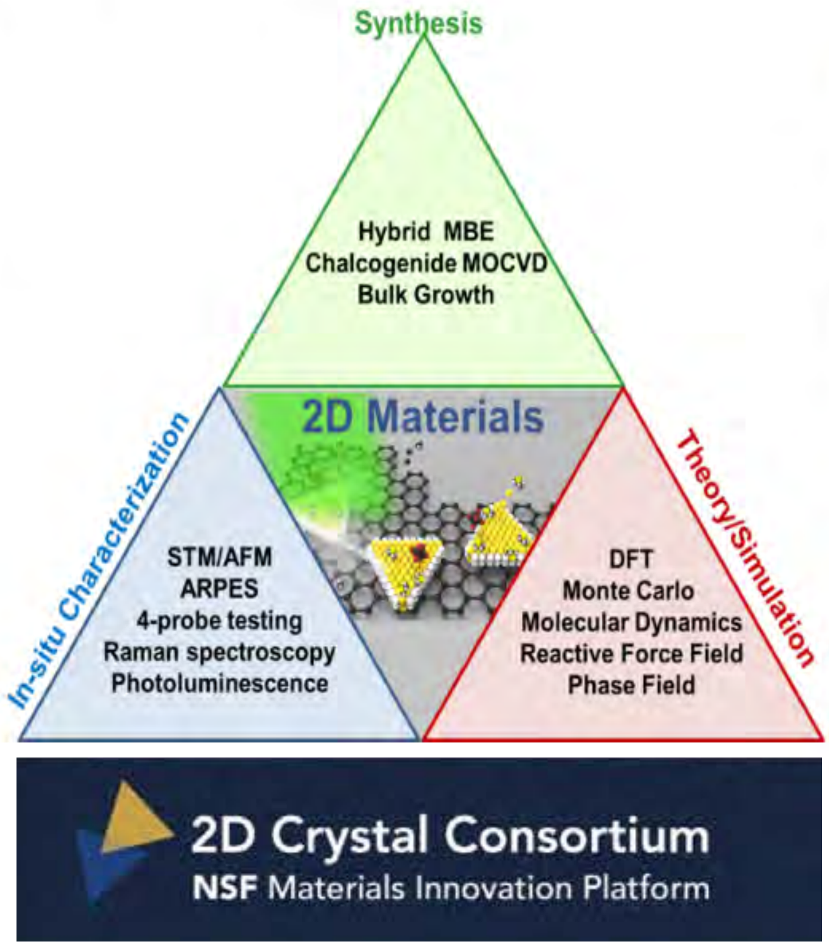
Jun Lou

SF Nanotech® 南京科孚纳米技术有限公司 Nanjing SCF Nanotech, Ltd

LOCKHE



Two New NSF-Funded Research Centers



Joan Redwing
Director

Nitin Samarth
Assoc. Director

Vincent Crespi
Theory Lead

Joshua Robinson
Director of User Programs

Eric Hudson
Director of Education

Kevin Dressler
Operations Director

PennState
Materials Research Institute

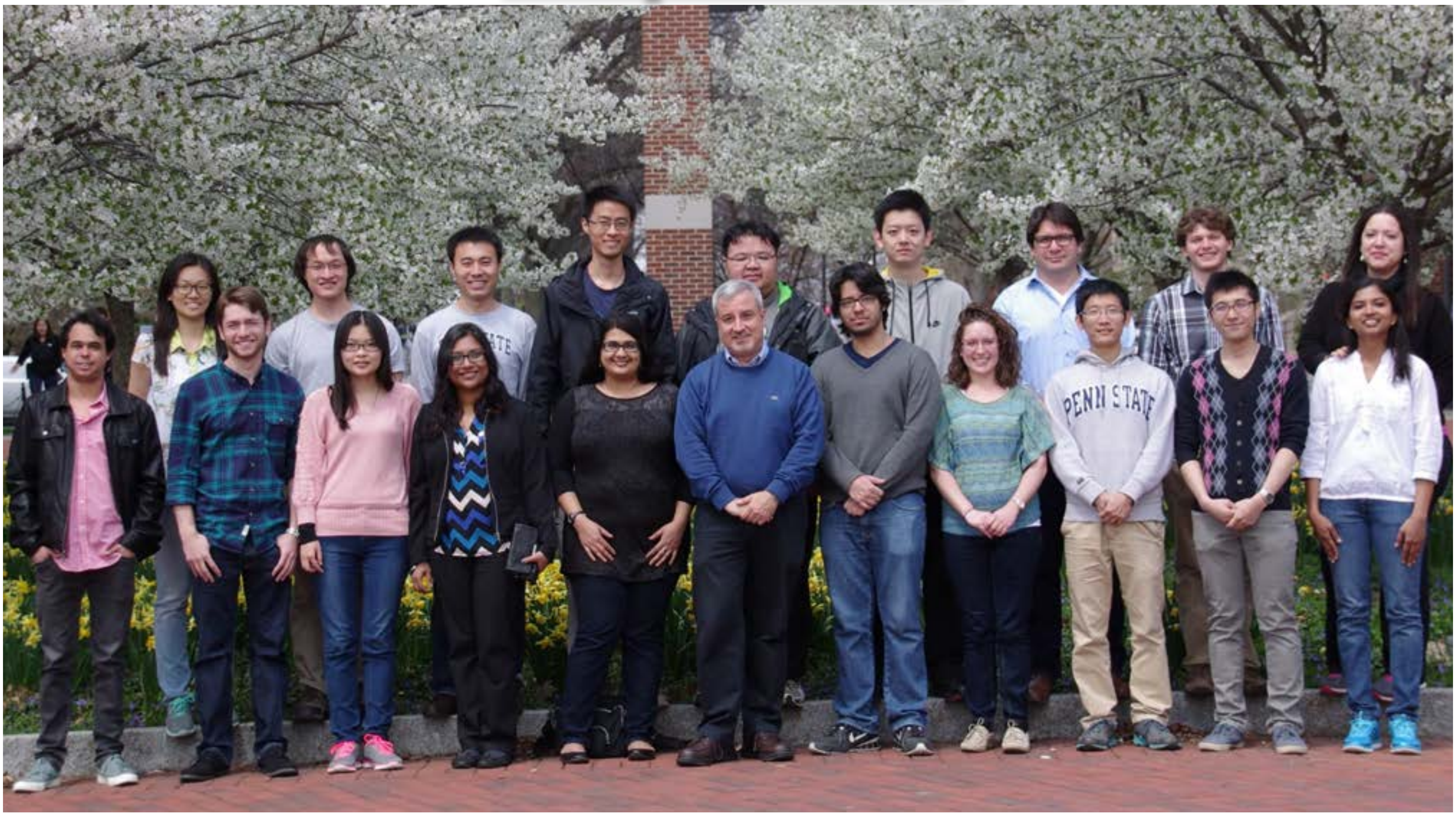
Center for Research on Advanced Fiber Technologies

CRAFT

Director
Melik C. Demirel
Co-Director
Mauricio Terrones

Center for 2-Dimensional and Layered Materials Penn State

Group Members



MURI Collaborators

- P.M. Ajayan (Rice University, USA)
- V.H. Crespi (PSU, USA)
- T.E. Mallouk (PSU, USA)
- S. Talapatra (USI-Carbondale, USA)
- B. I. Yakobson (RiceUniversity, USA)
- L. Balicas (Magnet Lab, USA)
- J. Lou (Rice University, USA)

- DoD Collaborators

  M. Dubey (ARL, USA)
  G. Birdwell (ARL, USA)
  F. Crowne (ARL, USA)
  M. Amani (ARL, USA)
  B. Maruyama (AFRL, USA)
  A. Roy (AFRL, USA)
  S. Karna (ARL, USA)

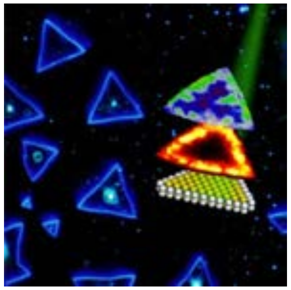
- Other Penn State Collaborators

  J. Robinson (MatScE)
  N. Samarth (Physics)
  J. Zhu (Physics)
  N. Alem (MatScE)
  T. Mayer (Engineering)
  Z.W. Liu (Engineering)

Center for 2-Dimensional and Layered Materials Penn State

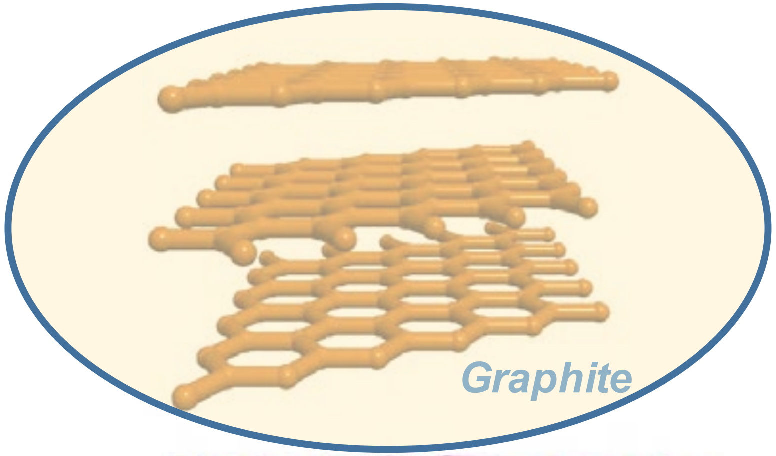
Layered Materials (1959)

What would the properties of materials be if we could really arrange the atoms the way we want them… I can hardly doubt that when we have some control of the arrangement of things on a small scale, we will get an enormously greater range of possible properties that substances can have…



R. P. Feynman
There is Plenty of Room at the Bottom
December 29, 1959

Perfect Layered Materials



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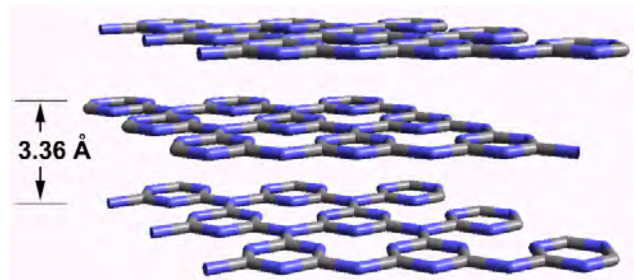
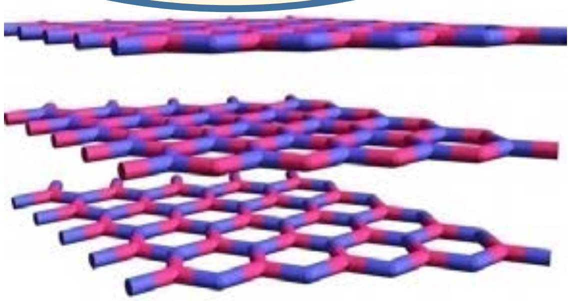
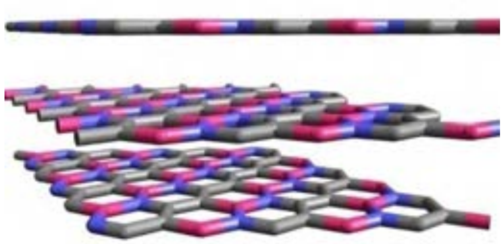


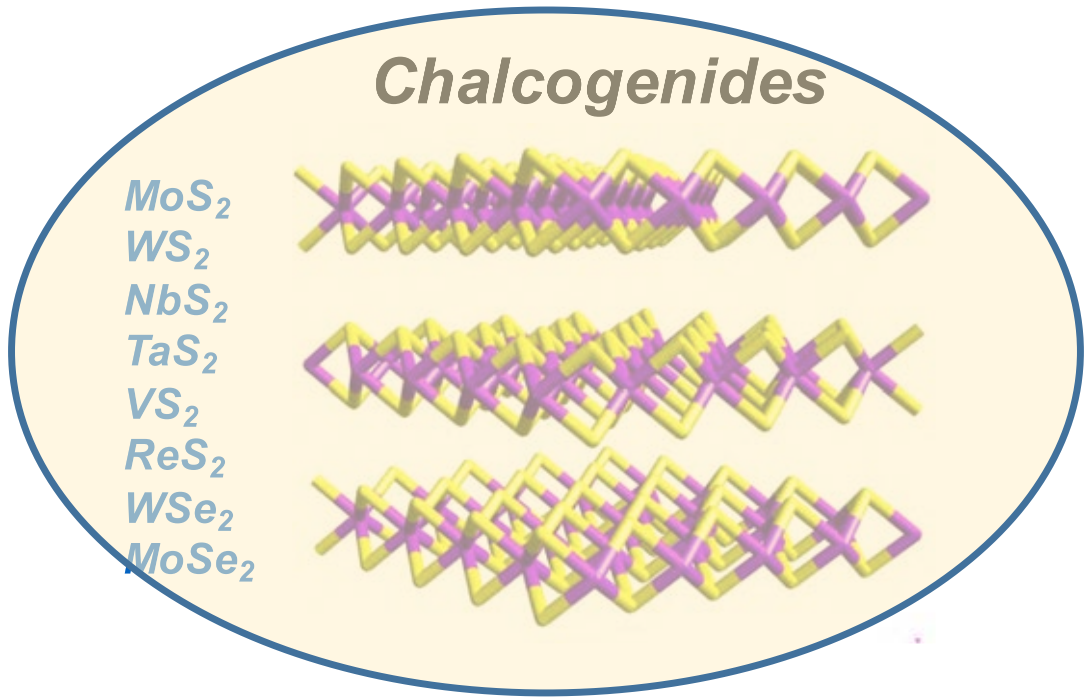
Carbon Nitride



Boron Nitride



Boron Carbo-Nitride



OTHERS VO_5, $NiCl_2$ MgB_2

Perfect Layered Materials

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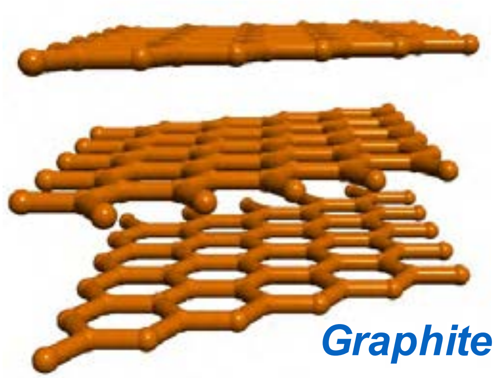
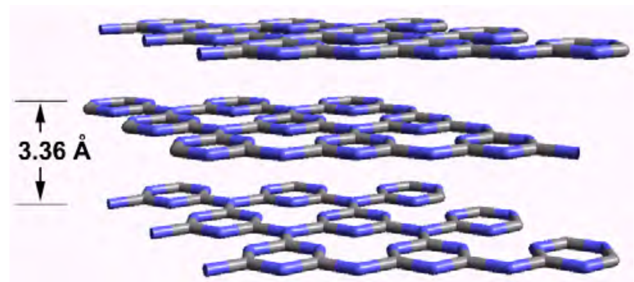
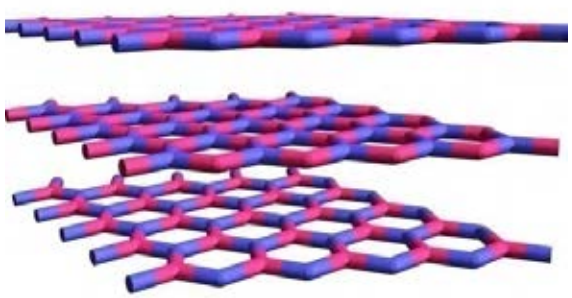


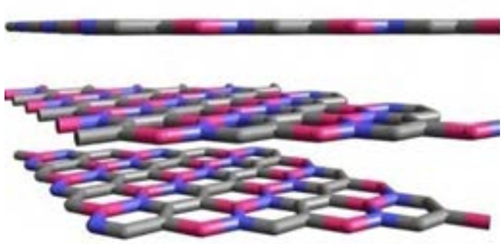
Graphite



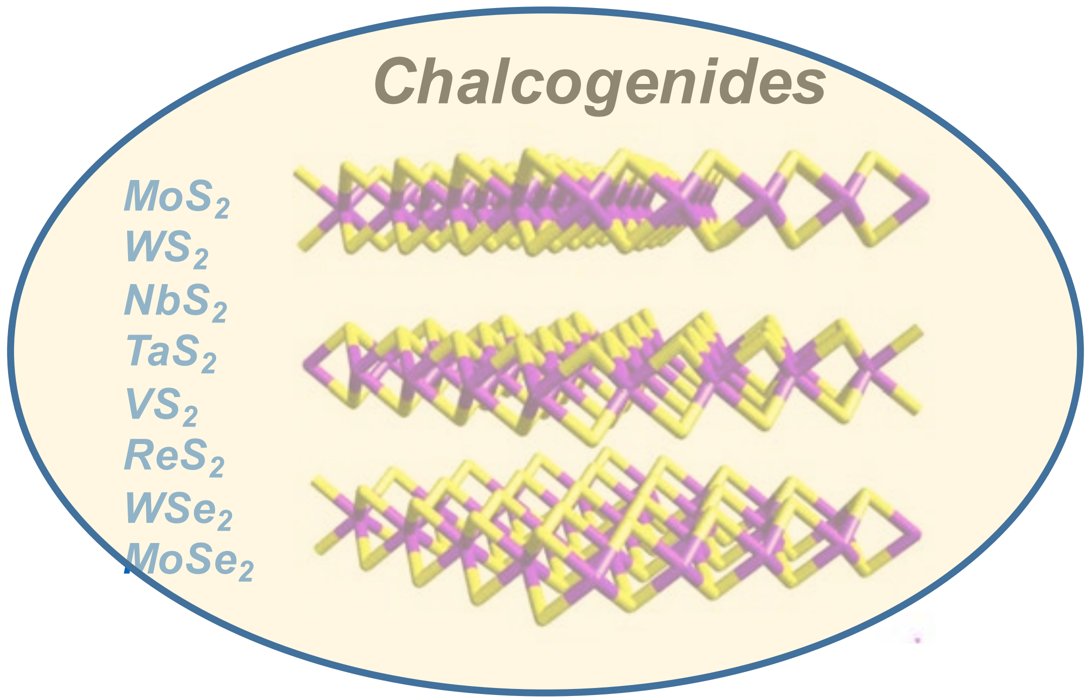
Carbon Nitride



Boron Nitride



Boron Carbo-Nitride



OTHERS VO_5, $NiCl_2$ MgB_2

Single Crystals of MoS_2 Several Molecular Layers Thick

R. F. FRINDT*

Physics and Chemistry of Solids, Cavendish Laboratory, Cambridge, England

(Received 24 March 1965; in final form 18 June 1965)

J. Appl. Phys. **37**, 1928 (1966); doi: 10.1063/1.1708627

Early workers on electron diffraction prepared thin fragments of MoS_2[2,3]; however no direct thickness measurements were made. It is now well known that small MoS_2 crystals thin enough to be transparent in the electron microscope can be prepared by the stripping technique using adhesive tape. Crystals of

The called scotch tape method for exfoliating graphite

SINGLE-LAYER MoS_2

Per Joensen, R.F. Frindt, and S. Roy Morrison
Energy Research Institute
Department of Physics
Simon Fraser University
Burnaby, B.C., Canada V5A 1S6

Mat. Res. Bull., Vol. 21, pp. 457-461, 1986. Printed in the USA.

ABSTRACT

MoS_2 has been exfoliated into monolayers by intercalation with lithium followed by reaction with water. X-ray diffraction analysis has shown that the exfoliated MoS_2 in suspension is in the form of one-molecule-thick sheets. X-ray patterns from dried and re-stacked films of exfoliated MoS_2 indicate that the layers are randomly stacked. Exfoliated MoS_2 has been deposited on alumina particles in aqueous suspension, enabling recovery of dry exfoliated MoS_2 supported on alumina.

Book on Layered Materials:

Wieting T. K., Schluter, M. In Physics and Chemistry of Materials with Layered Structures, (ed E. Mooser) (D. Reidel, Boston, 1979). ISBN 90-277-0897-5

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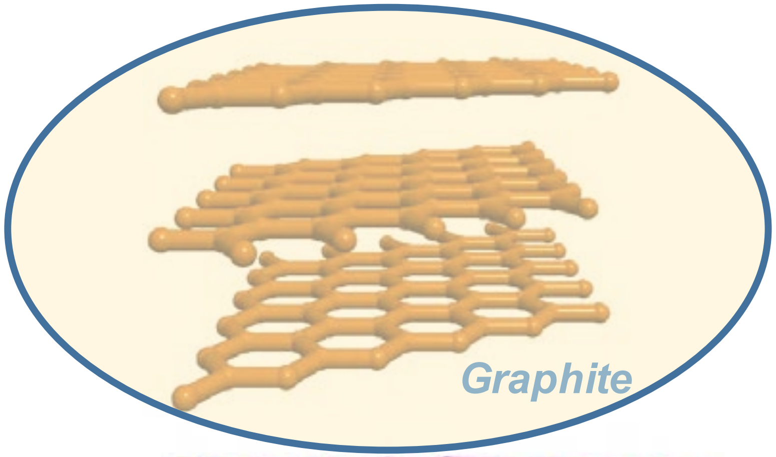
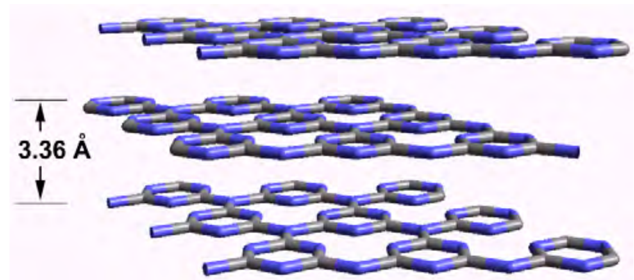
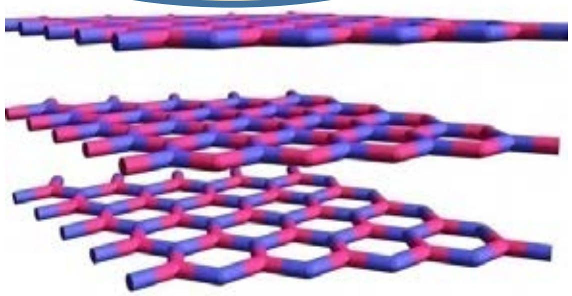
Layered Materials
Penn State

Perfect Layered Materials

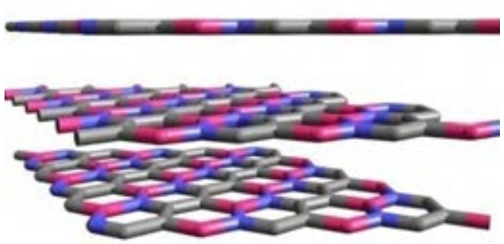




Carbon Nitride



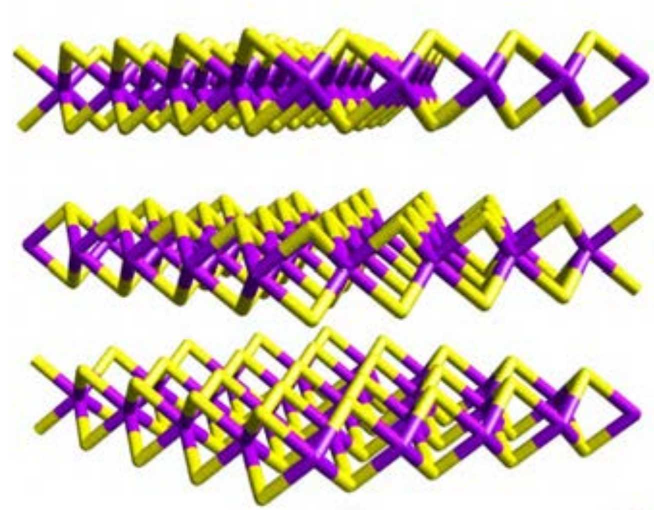
Boron Nitride



Boron Carbo-Nitride

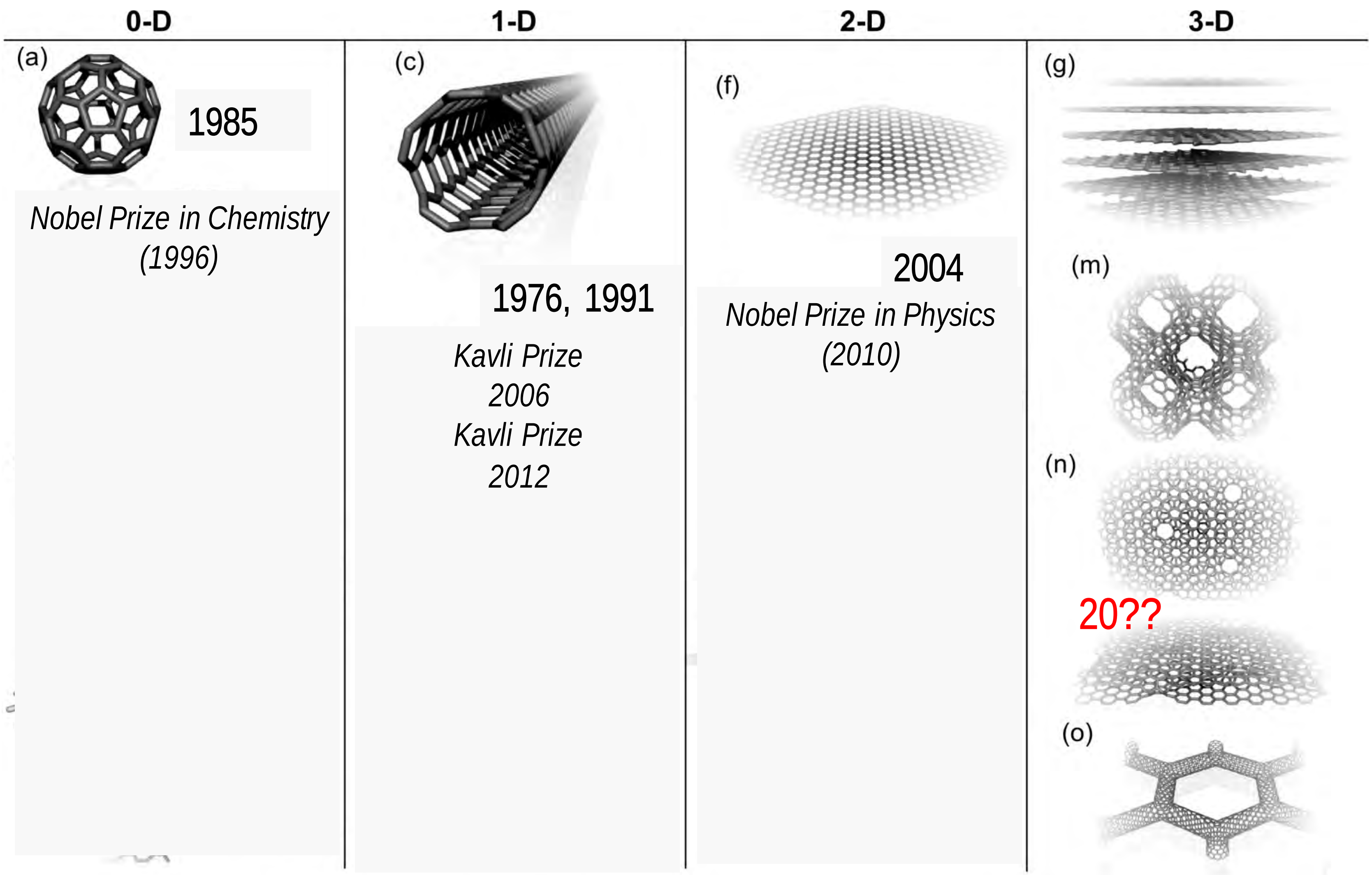
Chalcogenides

MoS_2
WS_2
NbS_2
TaS_2
VS_2
ReS_2
WSe_2
$MoSe_2$



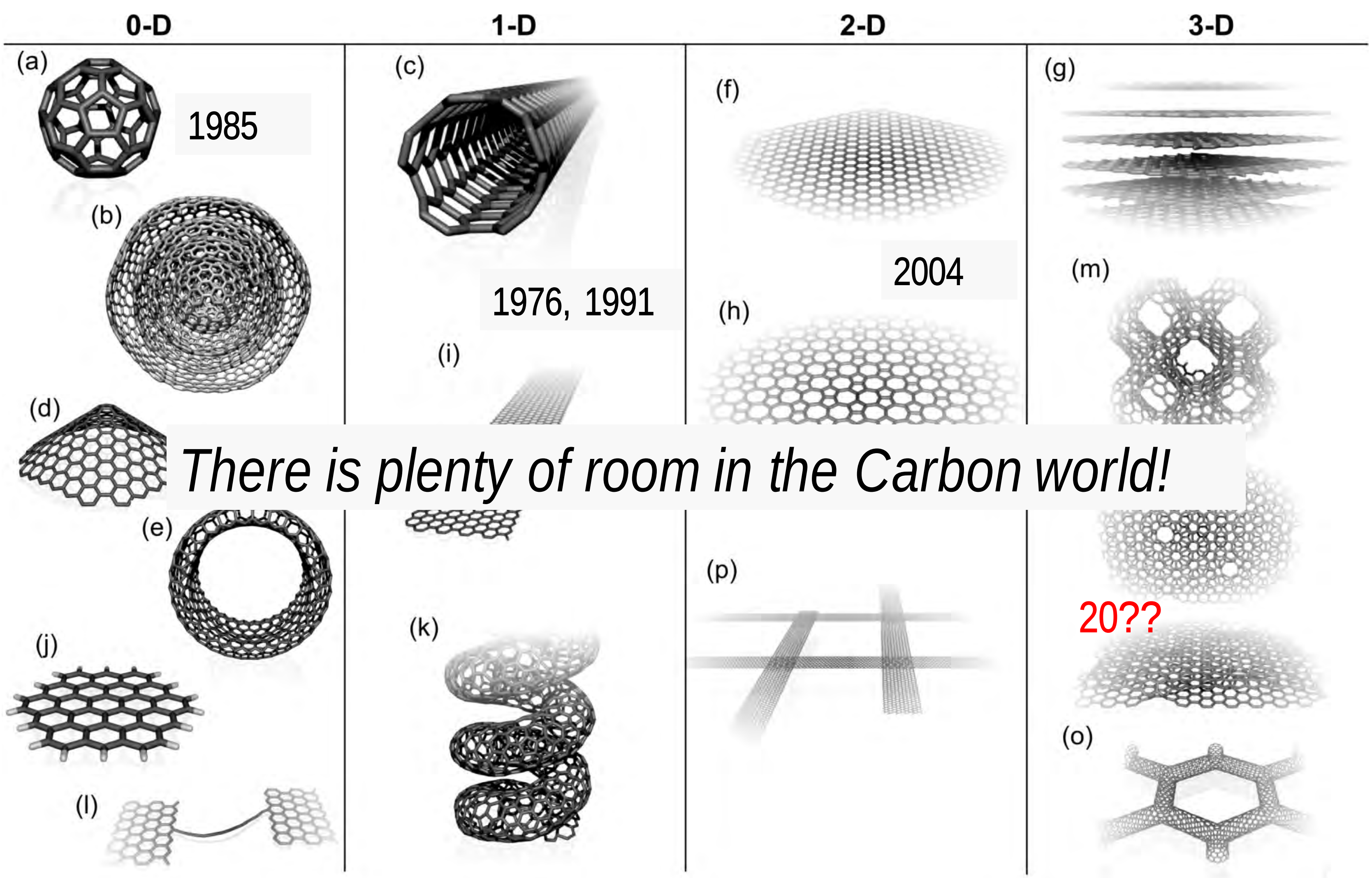
OTHERS VO_5, $NiCl_2$ MgB_2

NEW FORMS OF SP^2 CARBON



Terrones, M., et al. Nano Today 5, 351-372 (2010).

NEW FORMS OF SP^2 CARBON



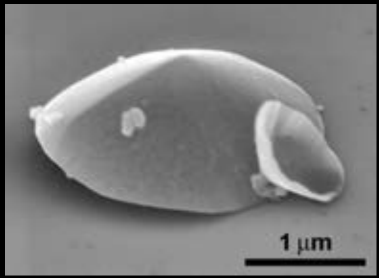
There is plenty of room in the Carbon world!

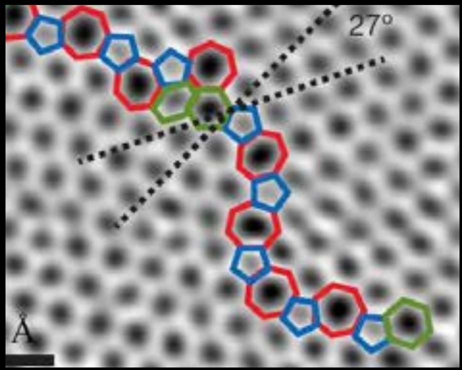
Terrones, M., et al. Nano Today 5, 351-372 (2010).

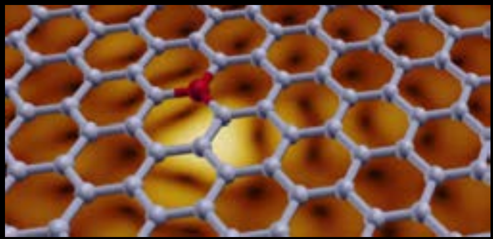
Other Forms of sp and sp^3 Carbon

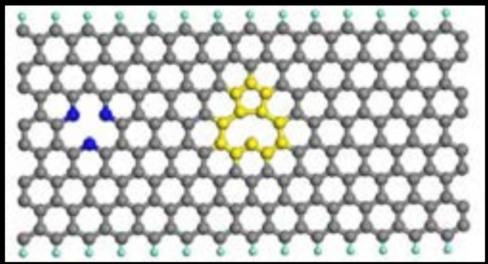
Defects in Graphene

1. Structural Defects, responsible of Curvature Changes (Pentagons, Heptagons, etc.)
2. Topological Defects (Bond Rotations, Stone-Thrower-Wales Type Transformations)
3. Substitutional Atoms (Impurities, Doping)
4. Vacancies, Interstitials and Edges
5. Folding, Surface Distortions?









Defects in Graphene

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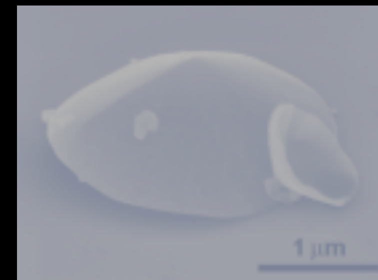
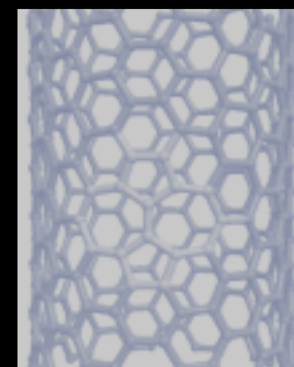
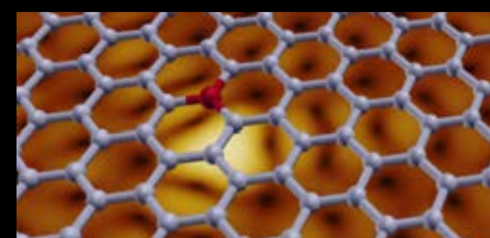
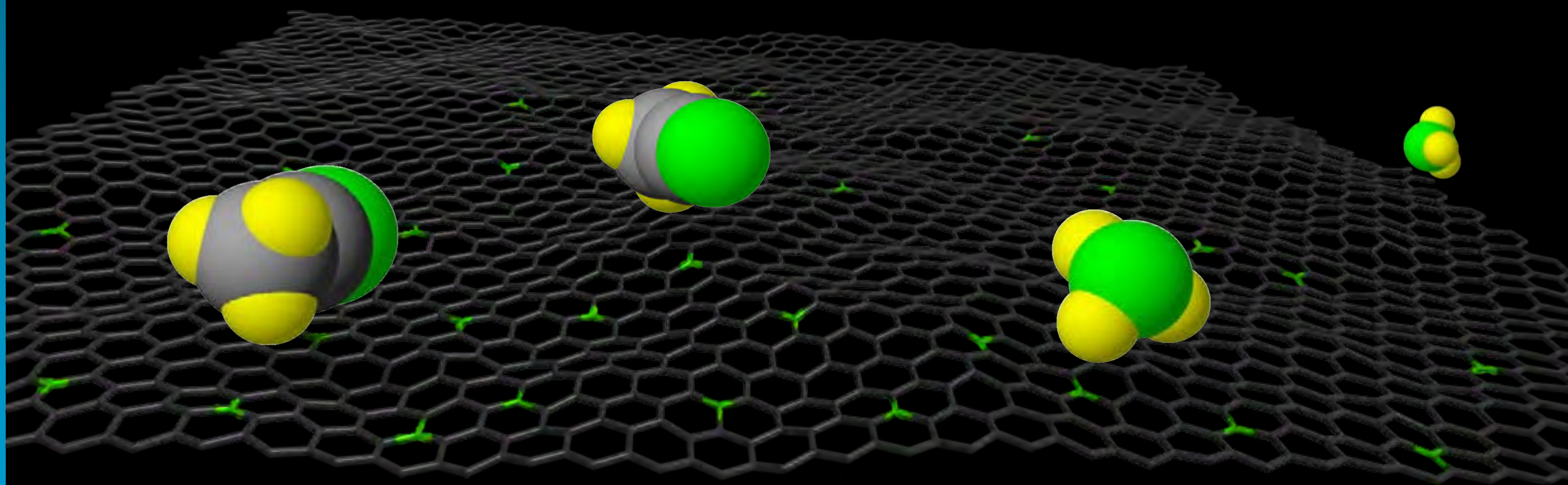


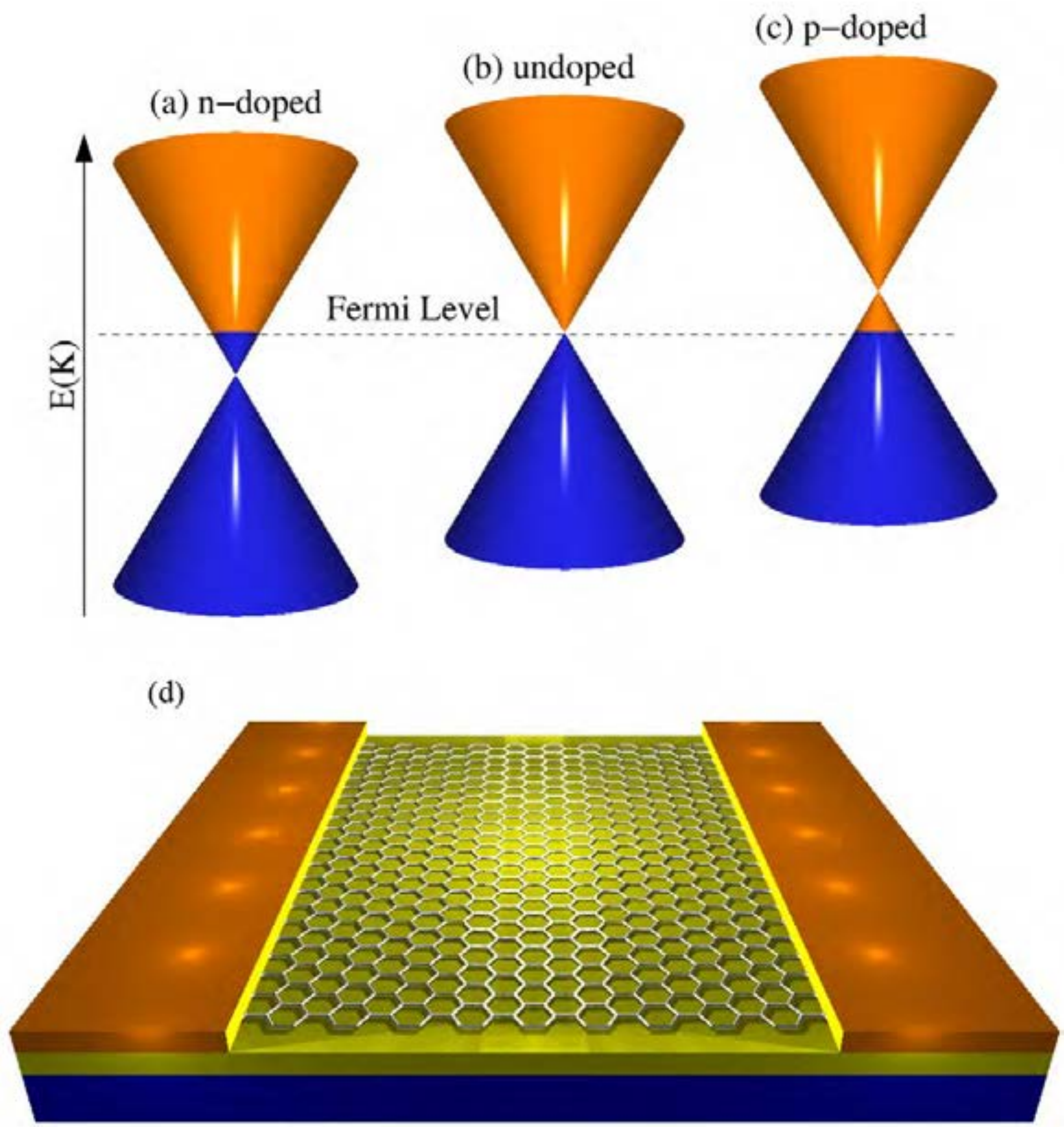




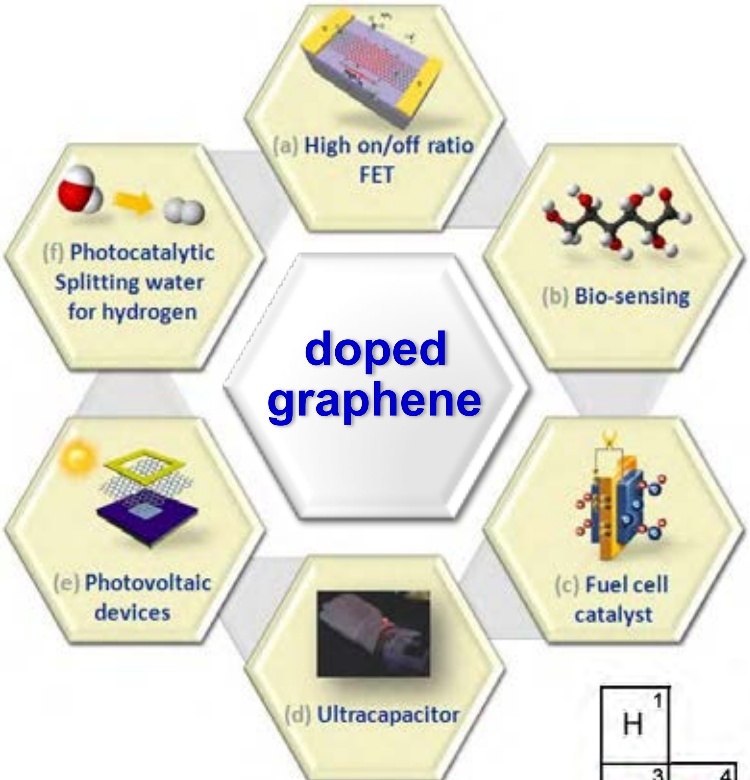
Doped Graphene



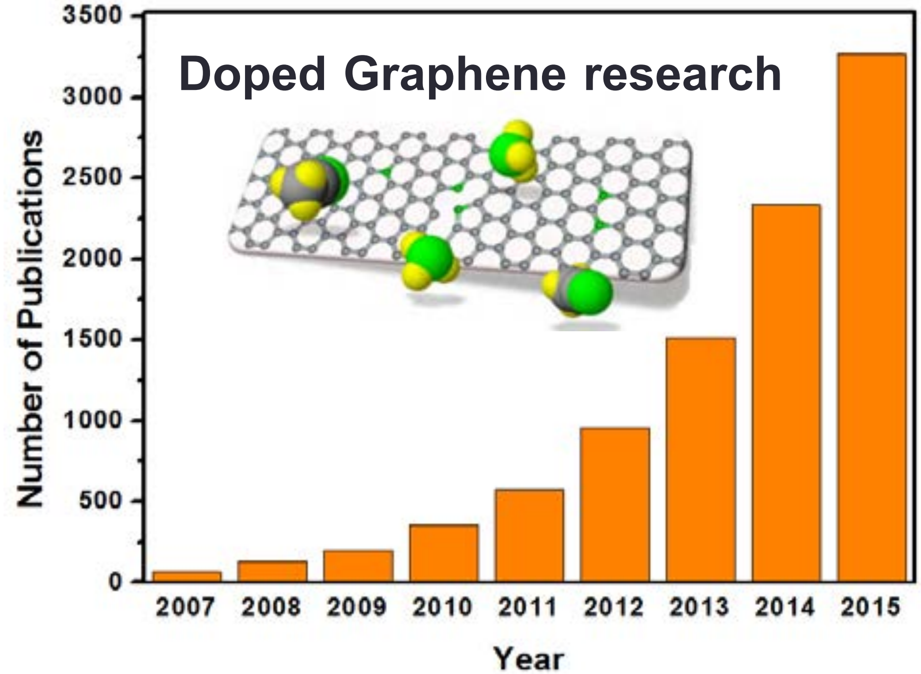
Fermi Level Shift in Graphene Caused by Doping: No Band Gap



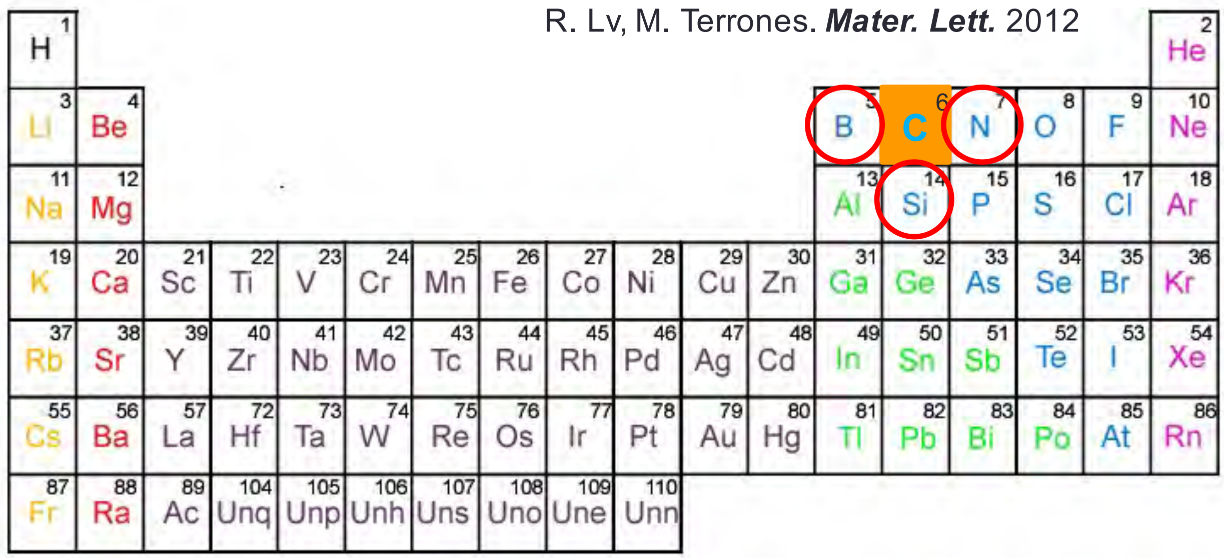
Doped Graphene Research



F. Lopez-Urias, R. Lv, M. Terrones. *Doped graphene: Theory, synthesis, characterization and applications*, **2013, Wiley**.



R. Lv, M. Terrones. ***Mater. Lett.*** 2012



Applications of N-doped graphene (NG)

- **High-frequency FET**

  Wang XR, *et al*. ***Science***, 2009, 324: 768-771

- **Bio-sensing**

  Wang Y, *et al*. ***ACS Nano*** 2010, 4: 1790-1798

- **Metal-free fuel cell catalyst**

  Qu LT, *et al*. ***ACS Nano*** 2010, 4: 1321-1326

- **Ultracapacitors**

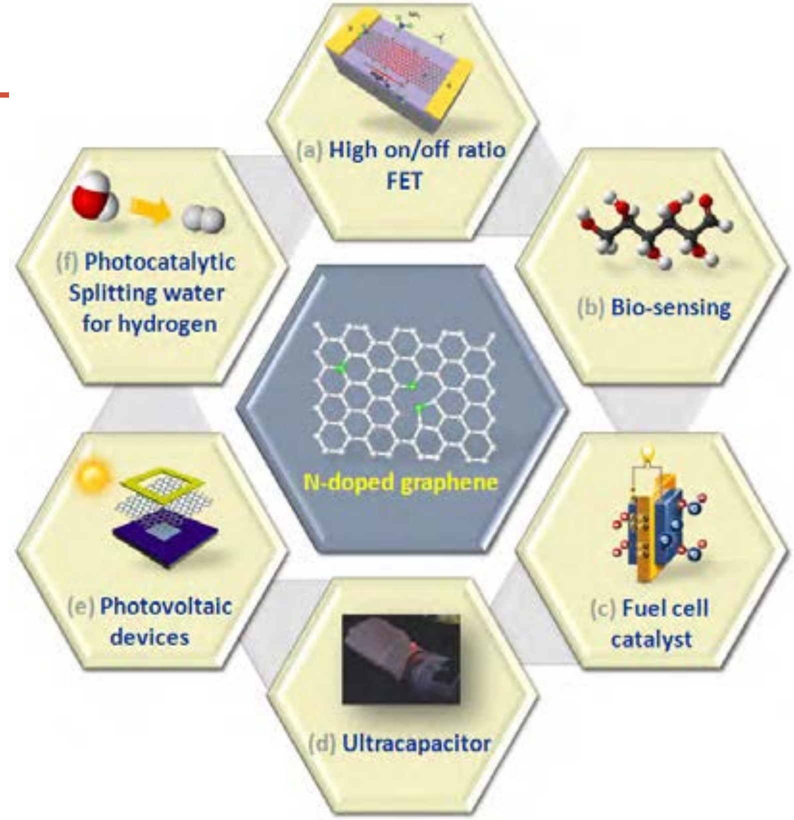
  Jeong HM, *et al*. ***Nano Lett***. 2011, 11: 2472-2477

- **Photovoltaic devices**

  Cui TX, *et al*. ***Carbon*** 2011, 49: 5022-5028

- **Photocatalytic splitting of water for hydrogen**

  Jia L, *et al*. ***J. Phys. Chem. C*** 2011, 115: 11466-11473



How nitrogen atoms are embedded in the graphene lattice?

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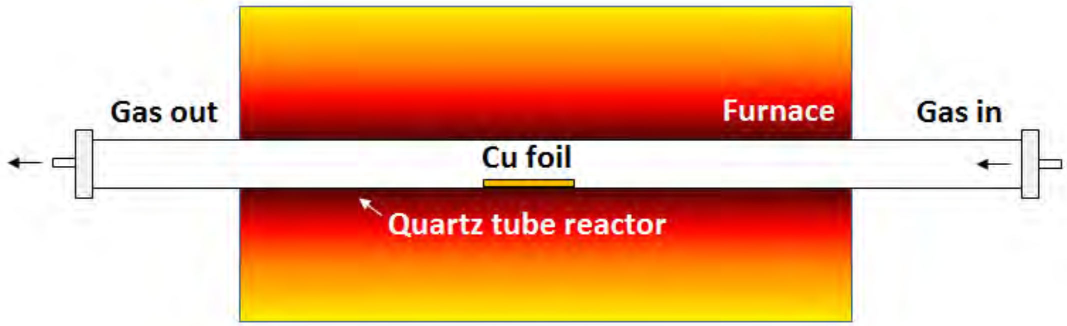
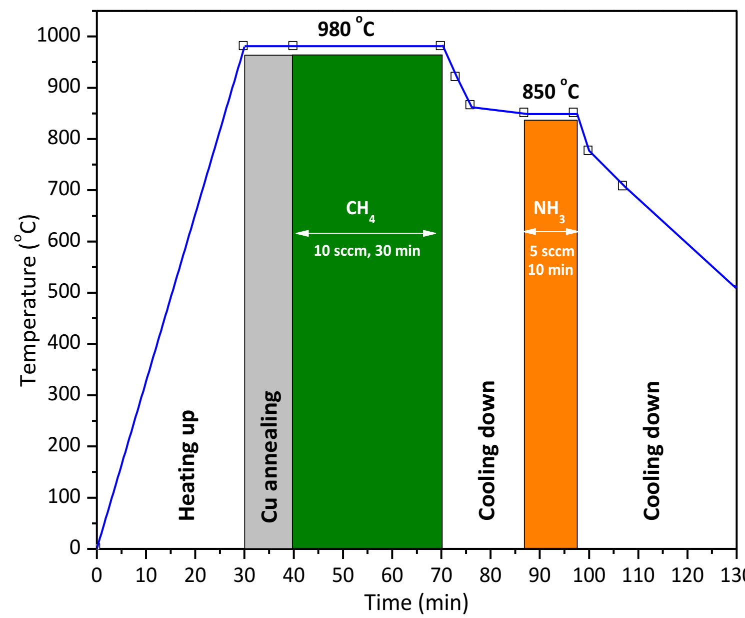
Growth of NG sheets from AP-CVD of this work



CH_4+Ar/H_2 (980°C)
NH_3 (850°C)

- ***Atmospheric-pressure*** ***chemical vapor deposition (AP-CVD)***
- ***Simple*** ***(No vacuum needed)***
- ***Efficient*** ***(Large-area, monolayer NG sheets could be obtained)***



R.T. Lv, et al., Nature Scientific Reports 2, 586 (2012).

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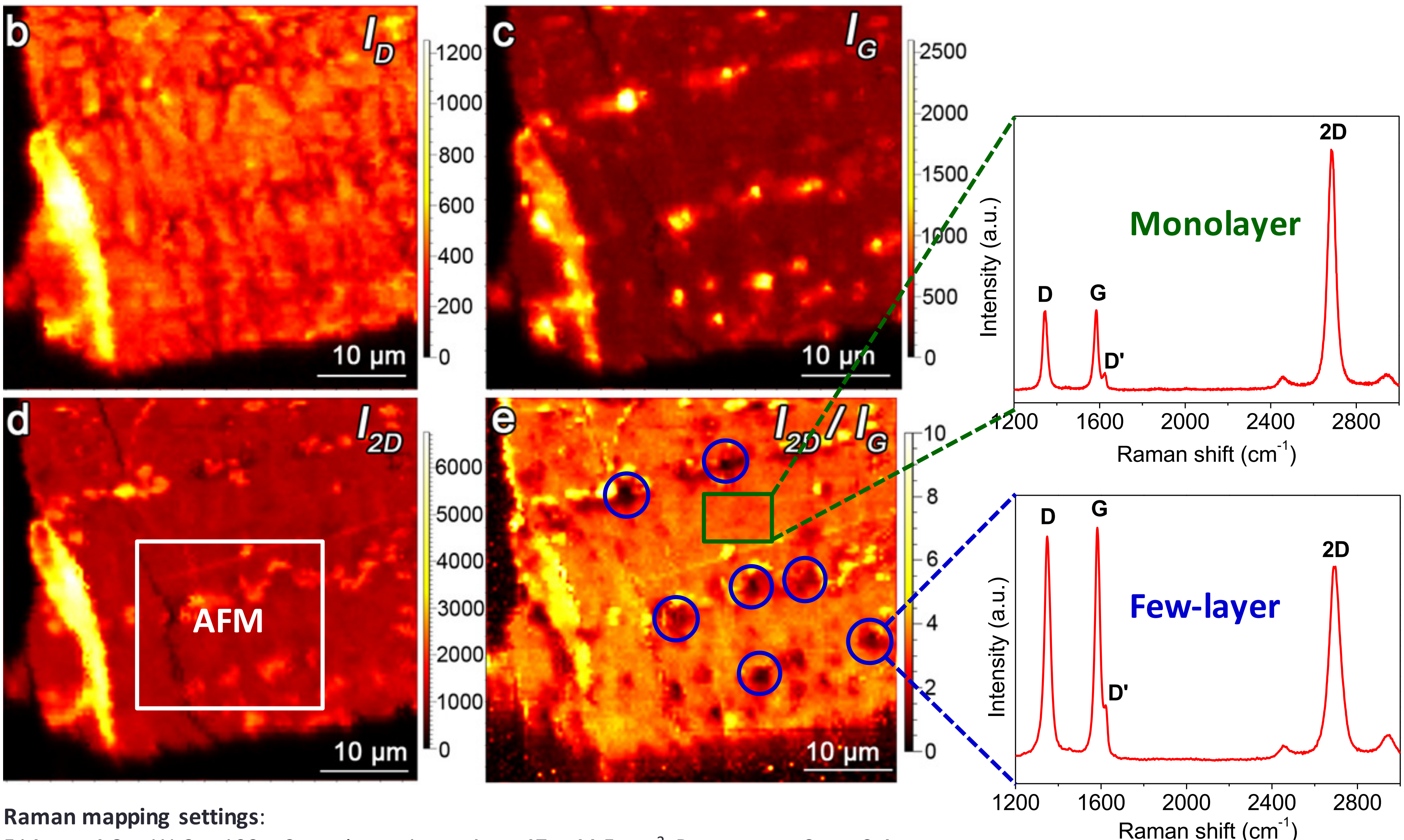
Raman mapping of NG sheet on SiO_2/Si substrate

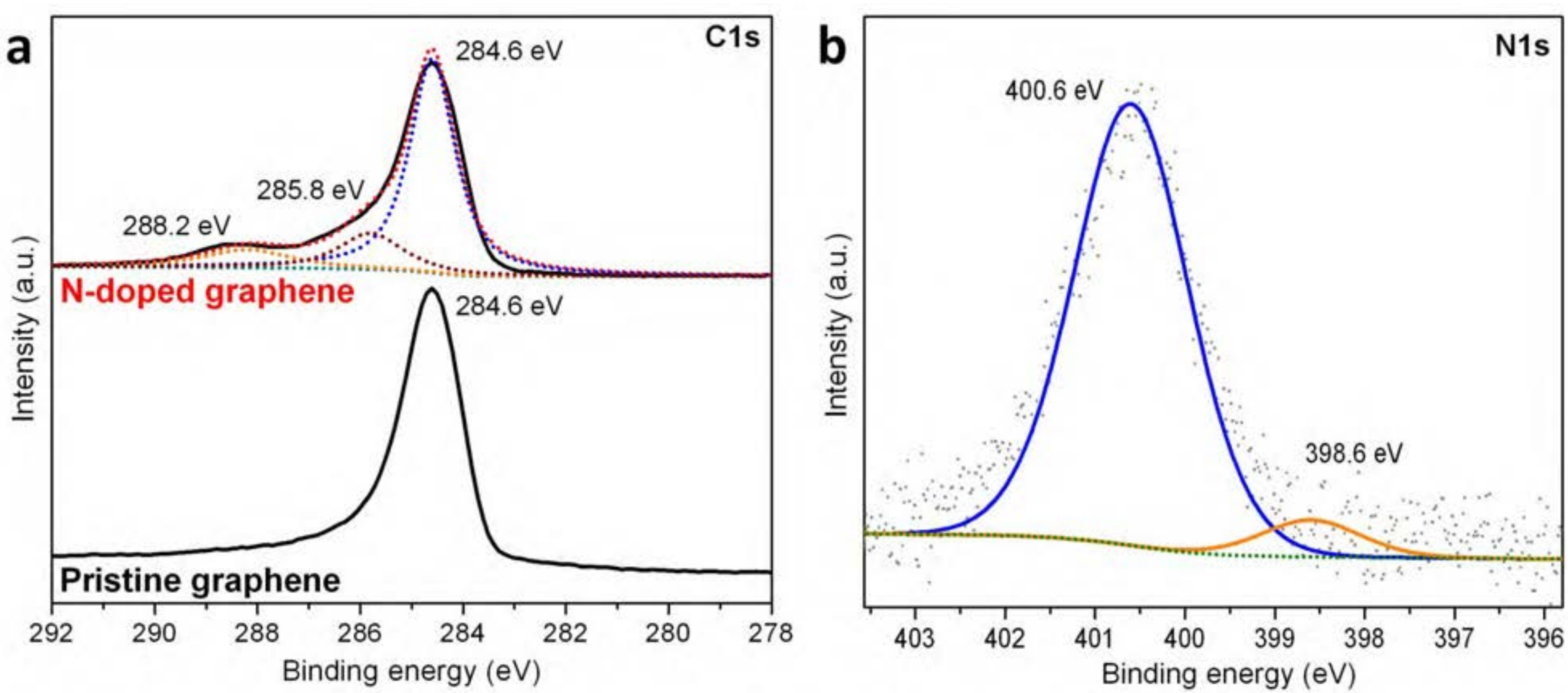


Raman mapping settings:
514 nm, 4.8 mW, 2 s, 100x, Spot size ≈ 1 μm, Area:47 x 44.5 μm^2, Raster scan, Step: 0.4 μm, Total 13,216 points,Time ≈ 18 hours

R.T. Lu, et al., Nature Scientific Reports 2, 586 (2012).

XPS spectra of NG and pristine graphene sheets

(XPS – X-ray Photoelectron Spectroscopy)



R.T. Lv, et al., Nature Scientific Reports 2, 586 (2012).

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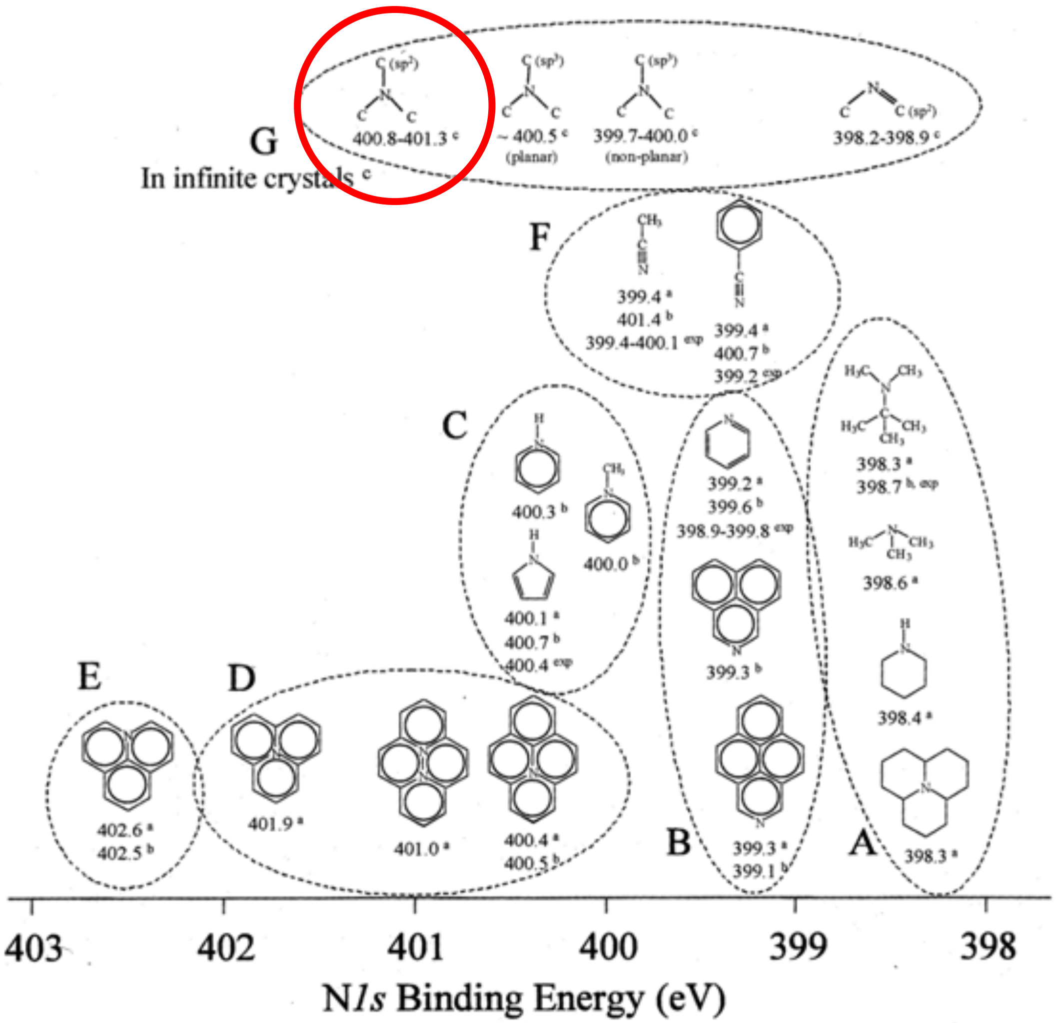
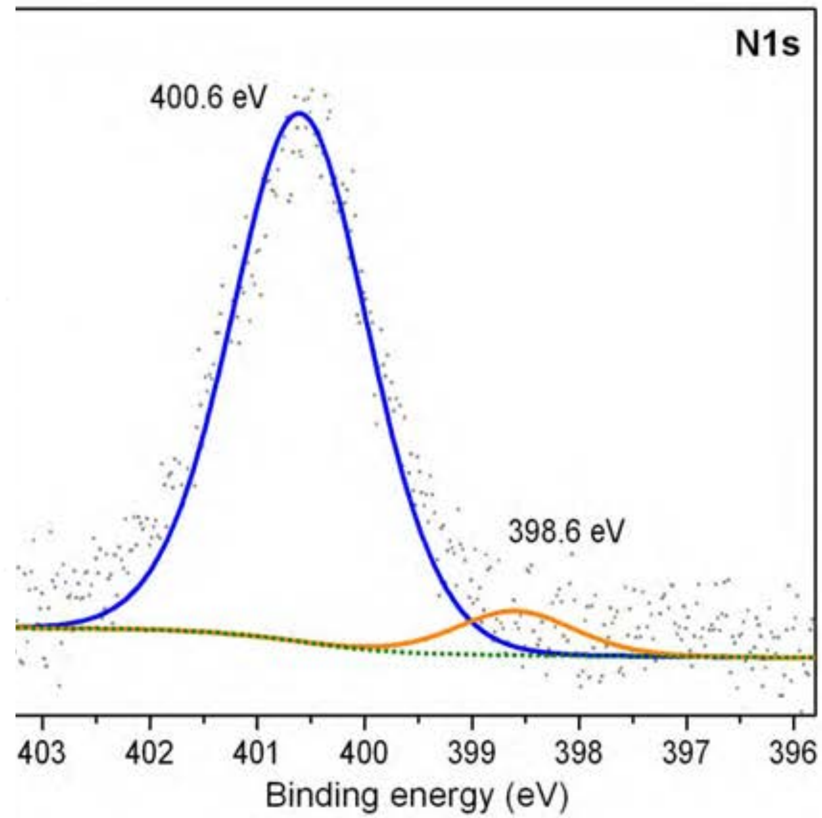
Calculated N1s binding energies for CNx structures

(XPS – X-ray Photoelectron Spectroscopy)





N. Hellgren, PhD. Thesis 1999 (Sweden)

R.T. Lu, et al., Nature Scientific Reports 2, 586 (2012).

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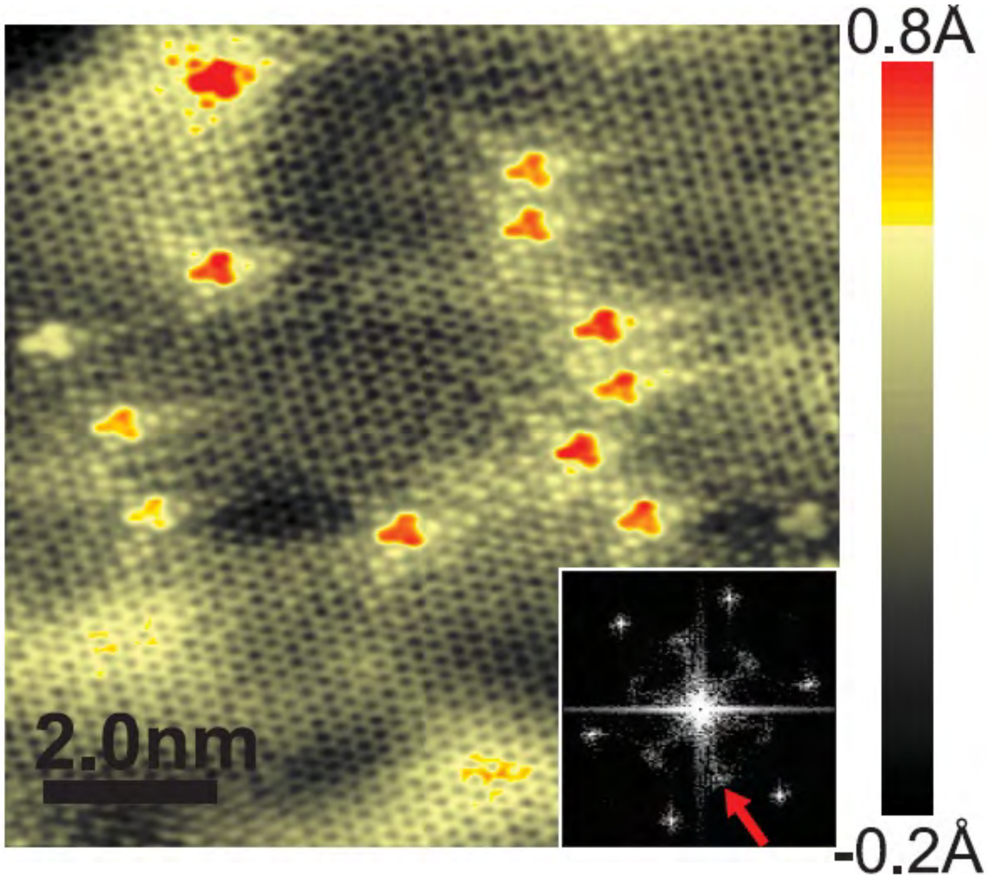
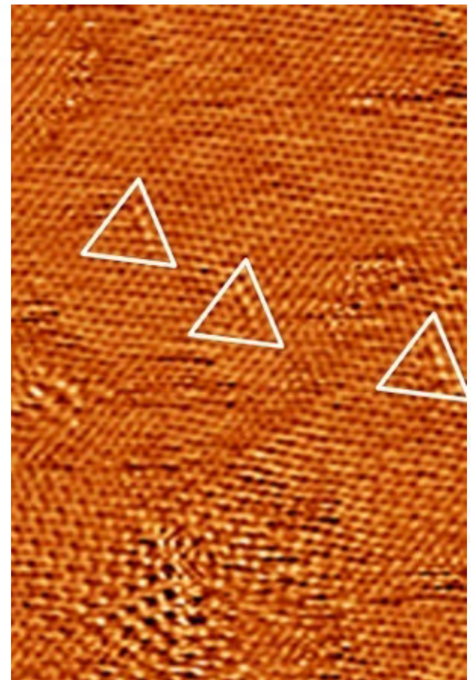
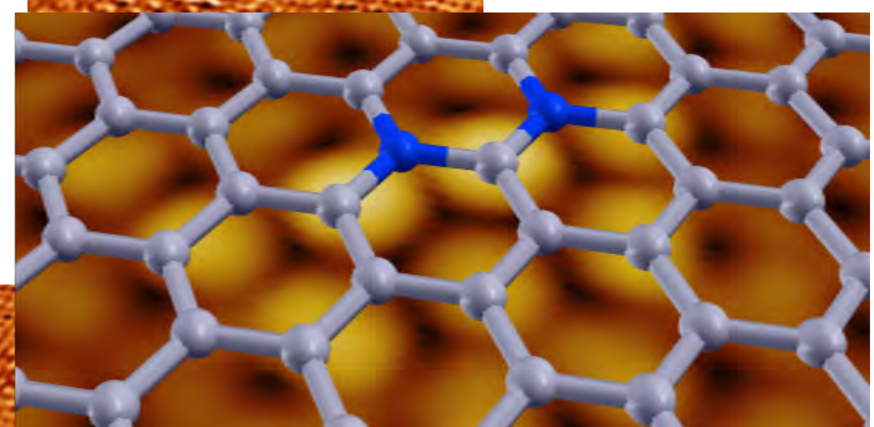
STM images of NG sheets on SiO_2/Si substrate

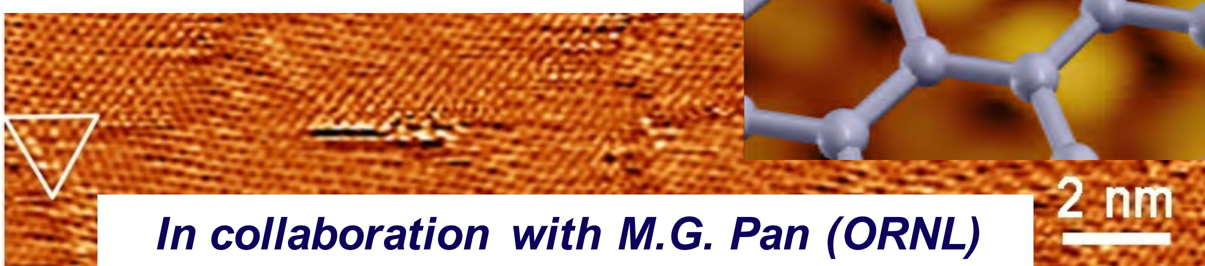
(STM – Scanning Tunneling Microscopy)



Zhao LY, *et al*. ***Science***, 2011, 333: 999-1003







In collaboration with M.G. Pan (ORNL)
A. Botello & J.C. Charlier (UCL)

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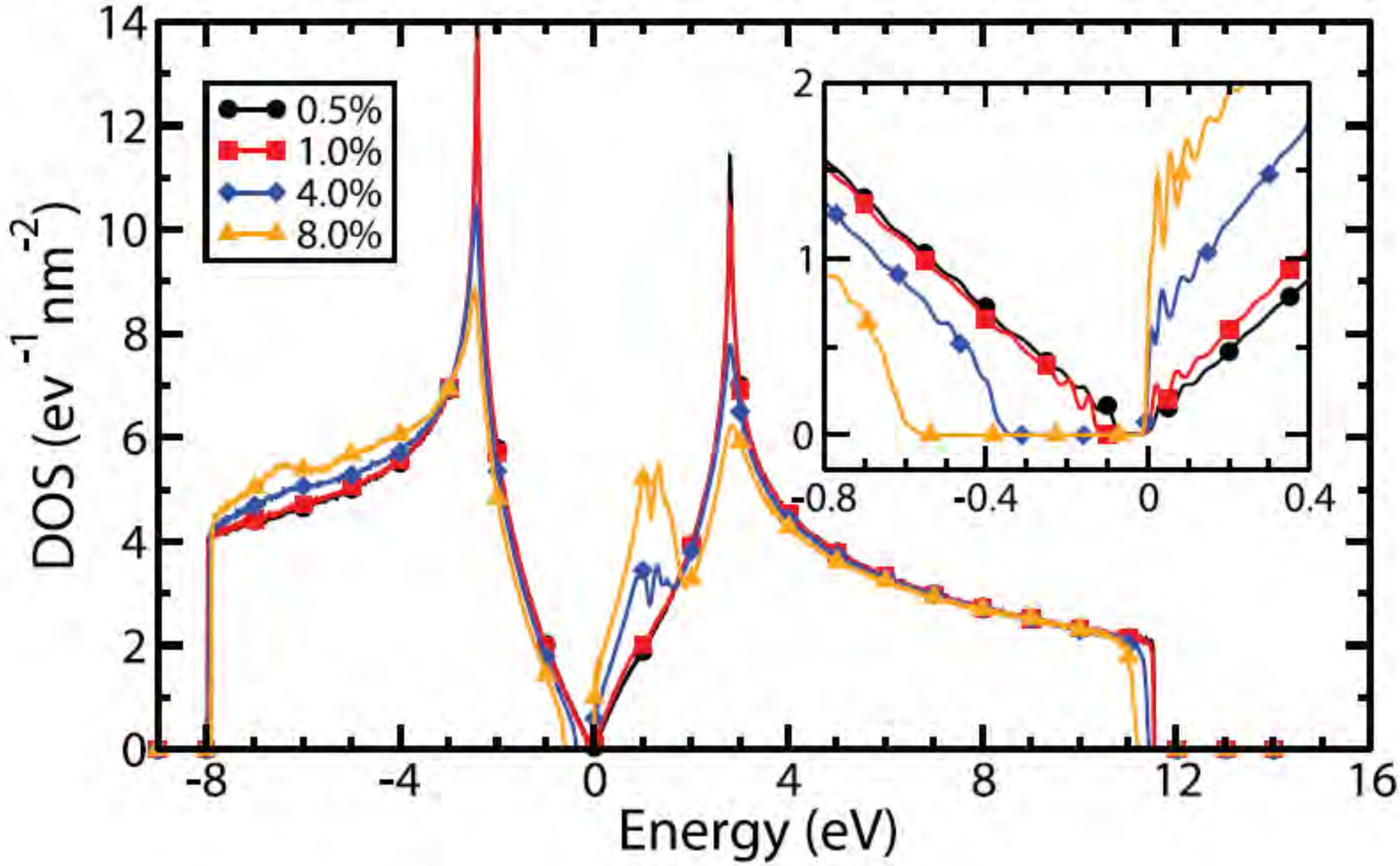
Band Gap Opening: Unbalanced Doping within Sublattices



A. Lherbier, A.R. Botello-Mendez & J.-C. Charlier, Nano Lett. (2013)

Lopez-Urias, et al., unpublished (2012)

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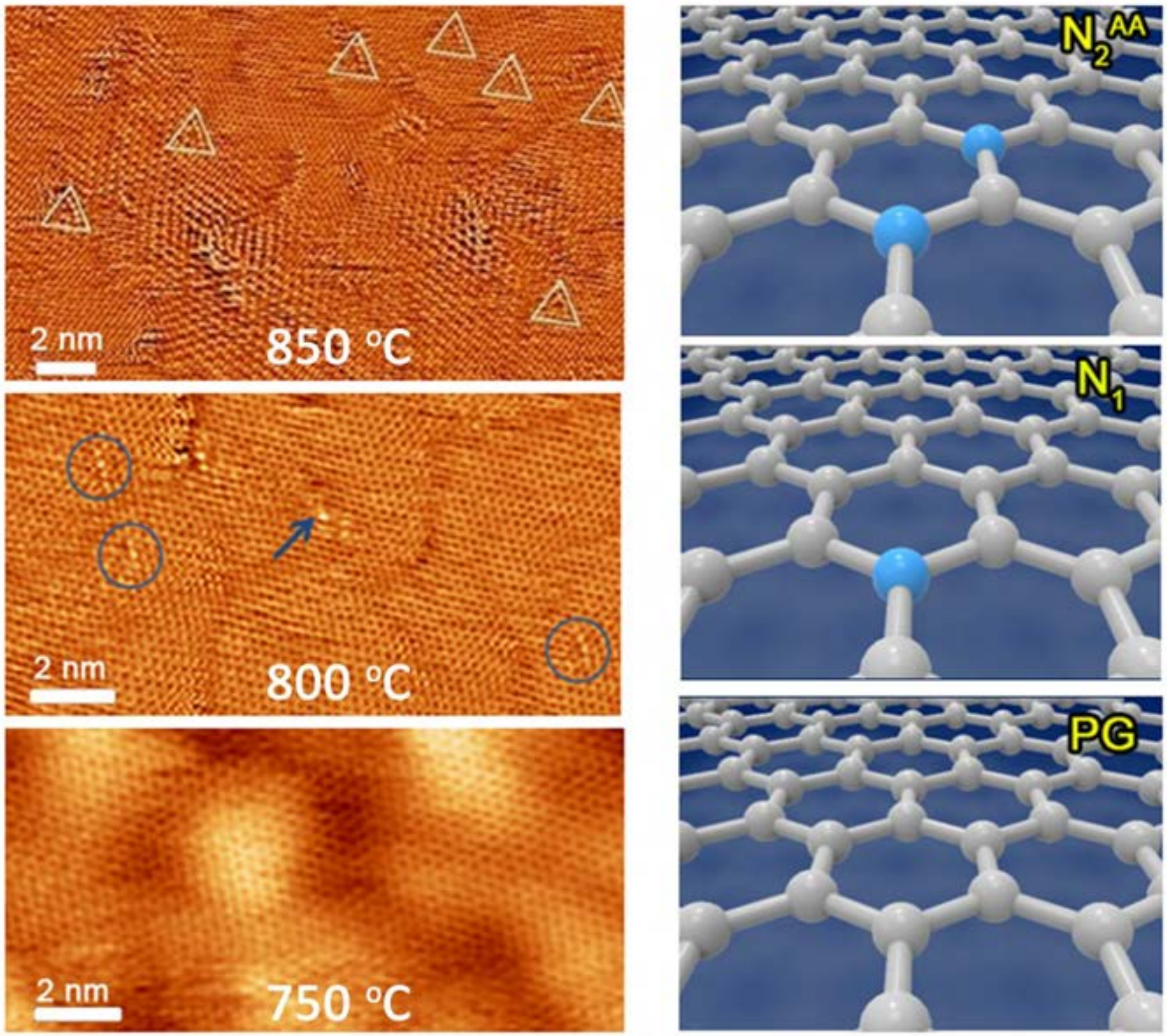
STM measurements on N-doped Graphene

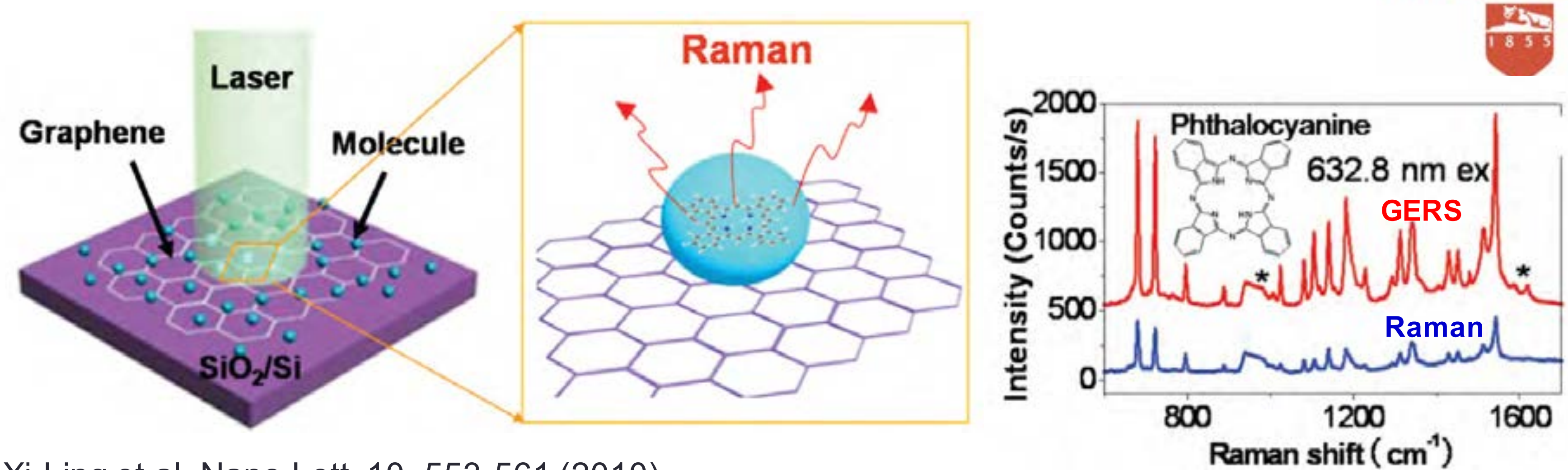
Tuning the N doping configurations by different synthesis conditions.



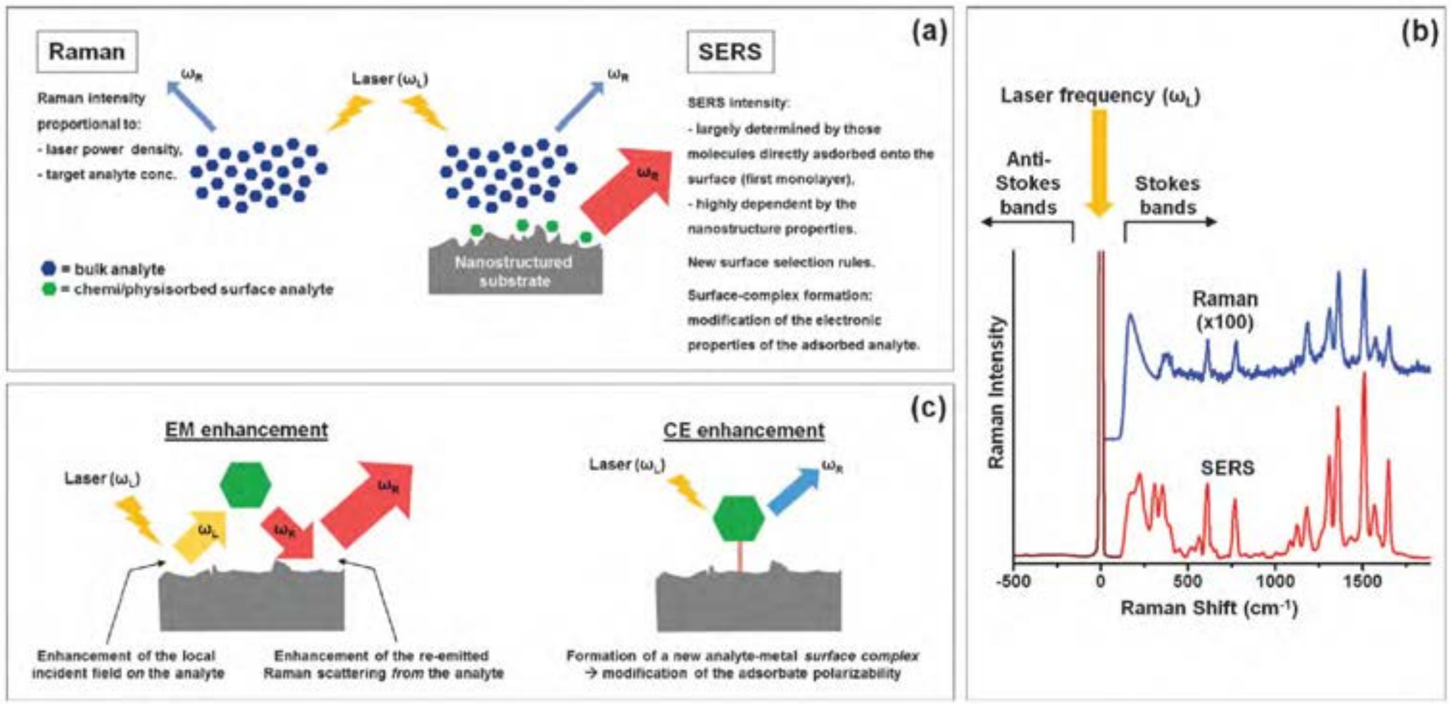
S. Feng, M. Terrones et al. ***Sci. Adv.* 2**, e1600322 (2016).

Mechanism of Graphene Enhanced Raman Scattering (GERS)

PENNSTATE



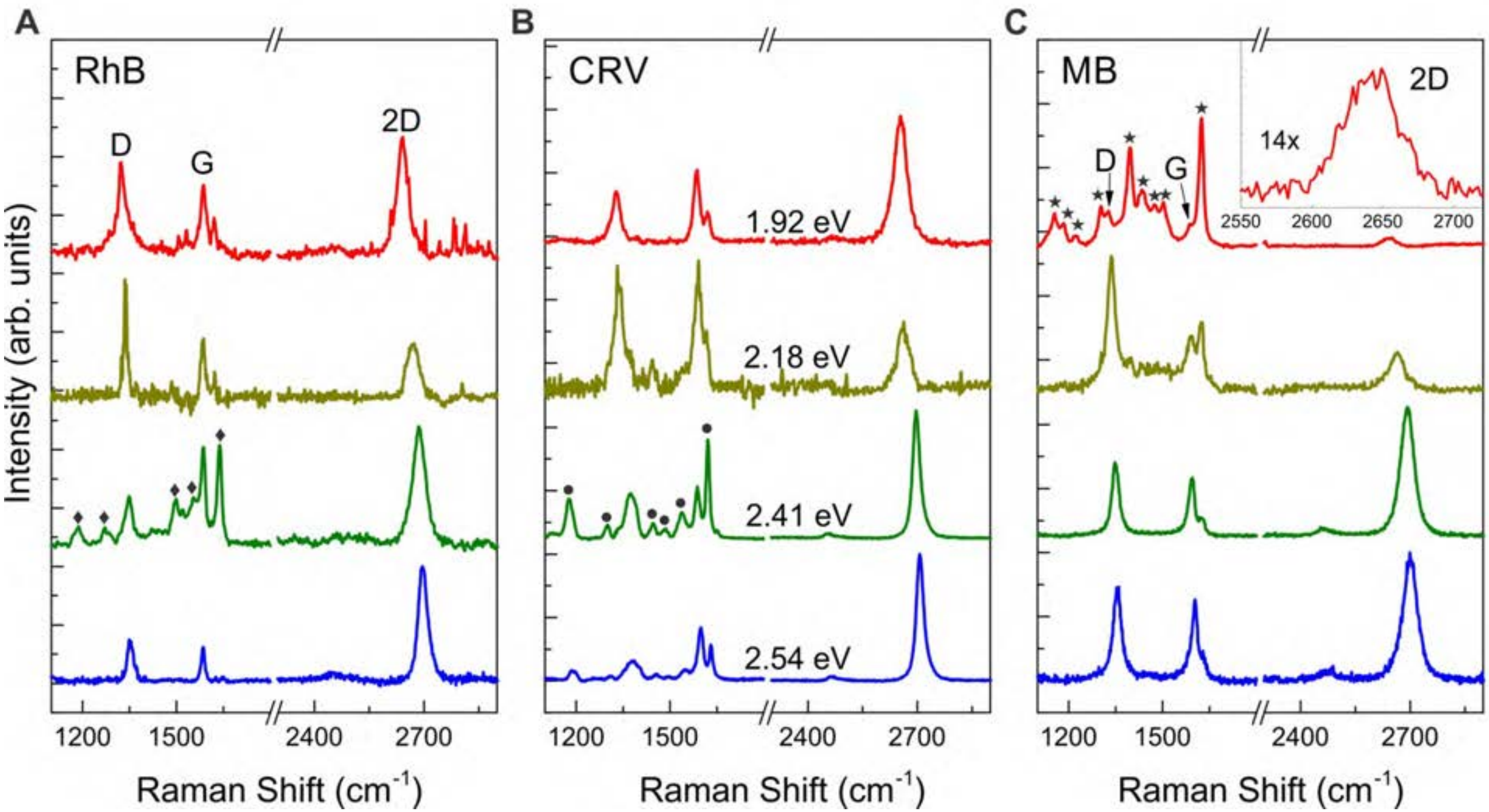
Xi Ling et al. Nano Lett. 10, 553-561 (2010)



Chem. Soc. Rev, ***41,*** *7085-7107 (2012)*

Mechanism of GERS on N-doped graphene

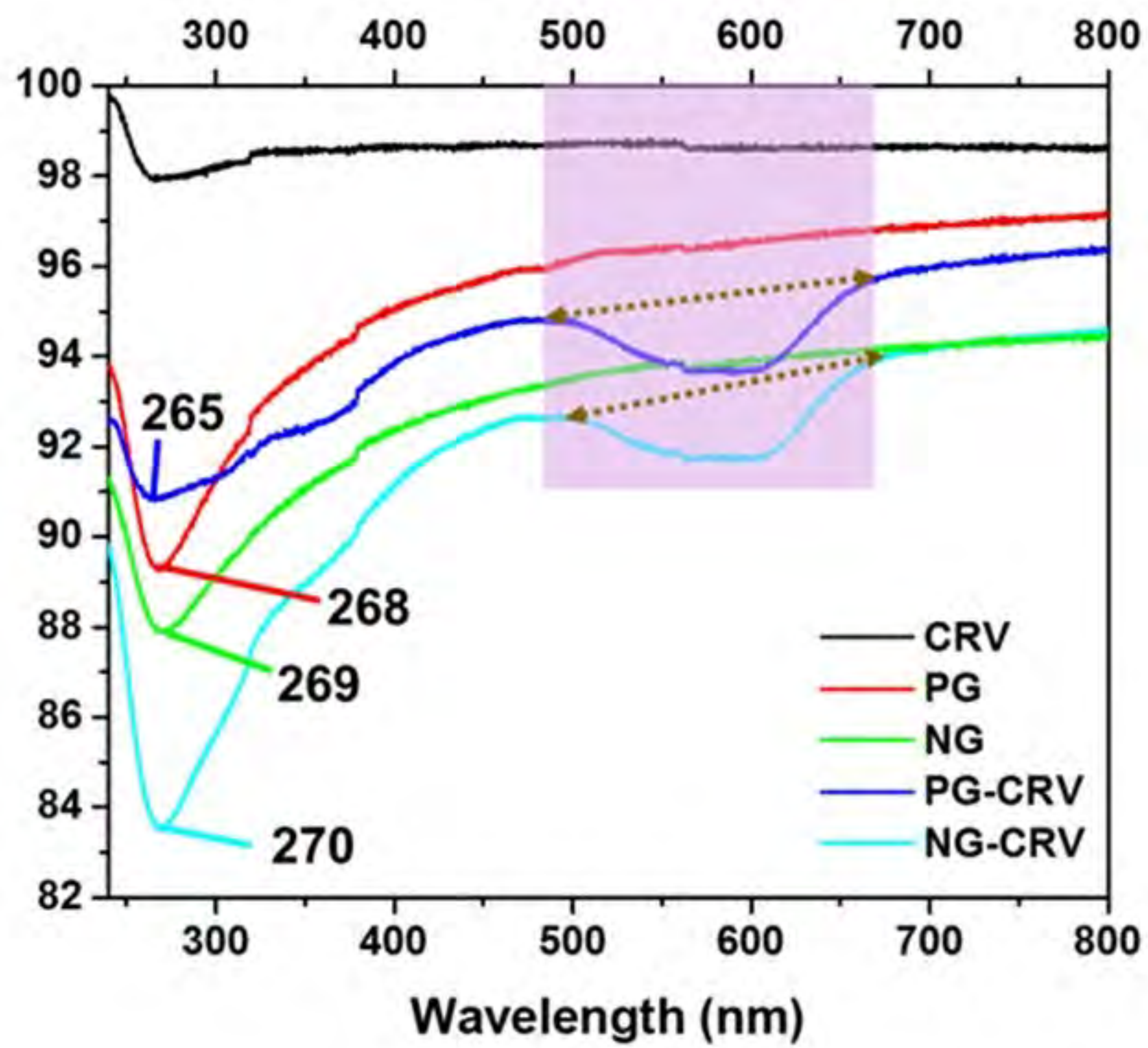
PENNSTATE



S. Feng, M. Terrones et al. ***Sci. Adv.*** **2**, e1600322 (2016).

Mechanism of GERS on N-doped graphene

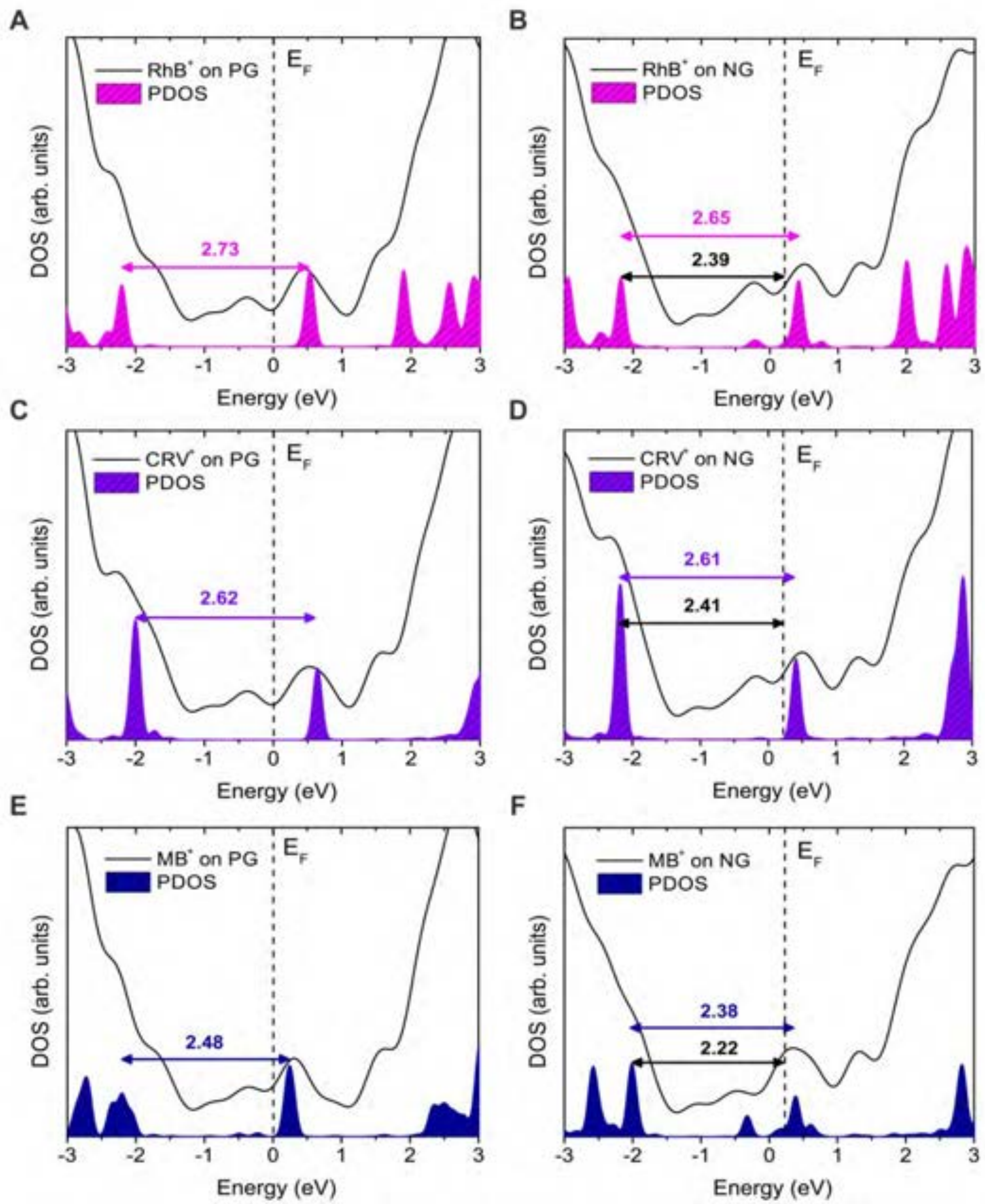
PENNSTATE



S. Feng, M. Terrones et al. ***Sci. Adv***. **2**, e1600322 (2016).

Mechanism of GERS on N-doped graphene

PENNSTATE



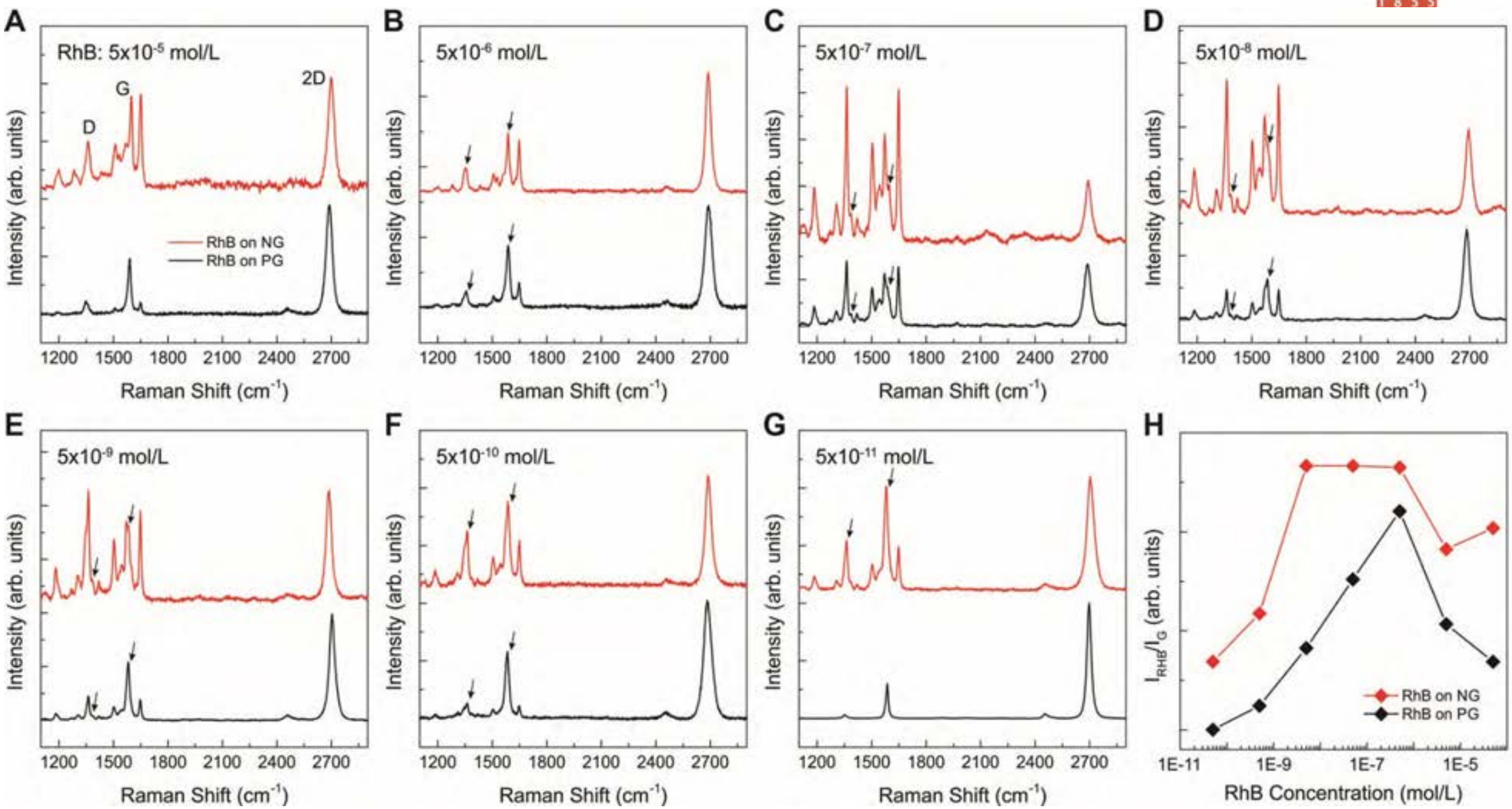
Dye	HOMO-LUMO gap on PG	HOMO-LUMO gap on NG	HOMO-E_F gap on NG	Adsorption peak	Resonant Laser energy
RhB	2.73 eV	2.65 eV	2.39 eV	2.29 eV	2.41 eV
CRV	2.62 eV	2.61 eV	2.41 eV	2.11 eV	2.41 eV
MB	2.48 eV	2.38 eV	2.22 eV	1.89 eV	1.92 eV

1. Charge-transfer mechanism
2. Fermi level should be close to LUMO of the molecules.
3. Molecular energy gap should be close to laser excitation energy.

S. Feng, M. Terrones et al. ***Sci. Adv*. 2**, e1600322 (2016).

Sensitivity of GERS on N-doped graphene

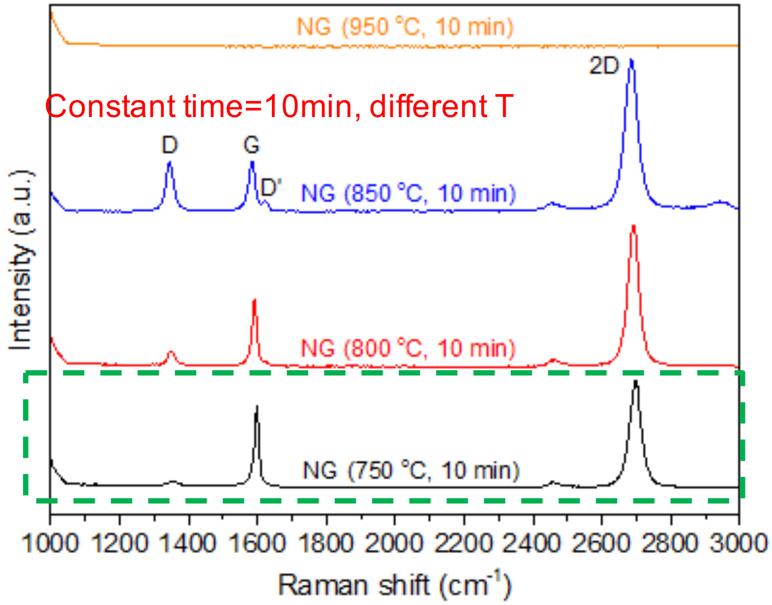
PENNSTATE

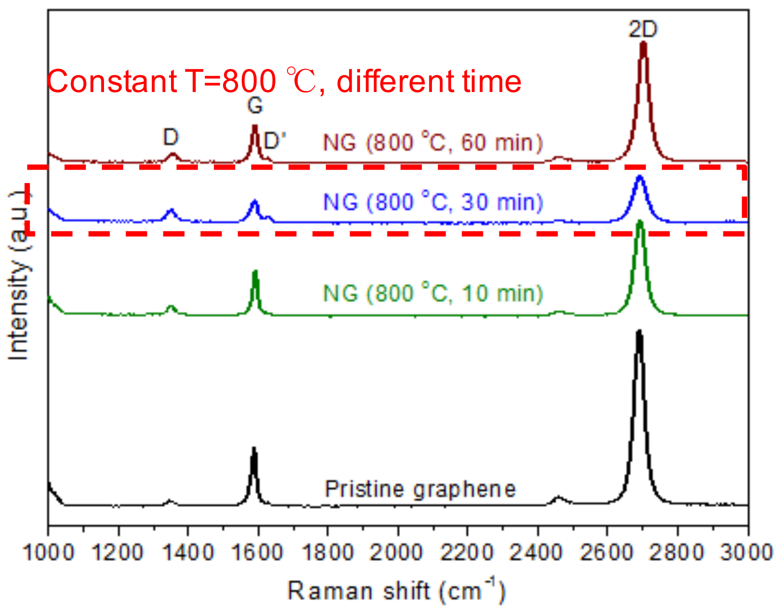


First time ever such low concentration could be detected with graphene as substrates.

S. Feng, M. Terrones et al. ***Sci. Adv.*** **2**, e1600322 (2016).

Tuning the doping level of N-doped graphene

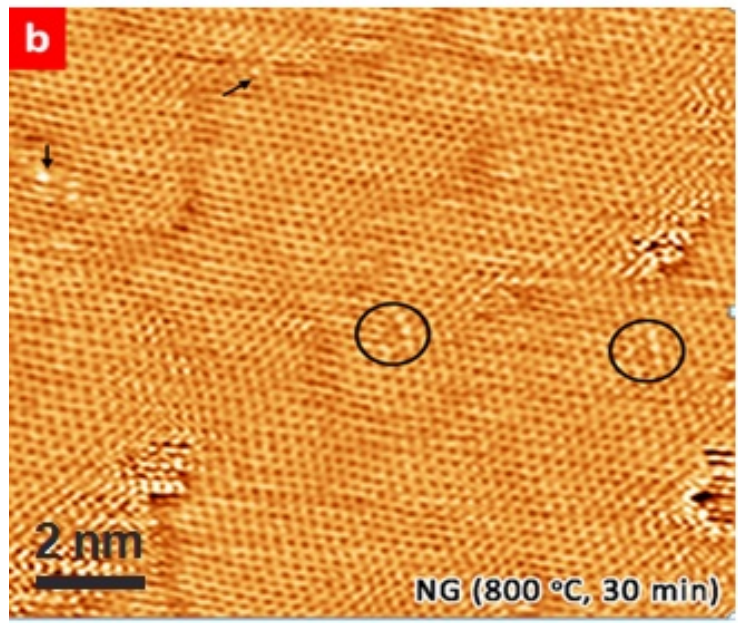




- **Question which remains for theory**

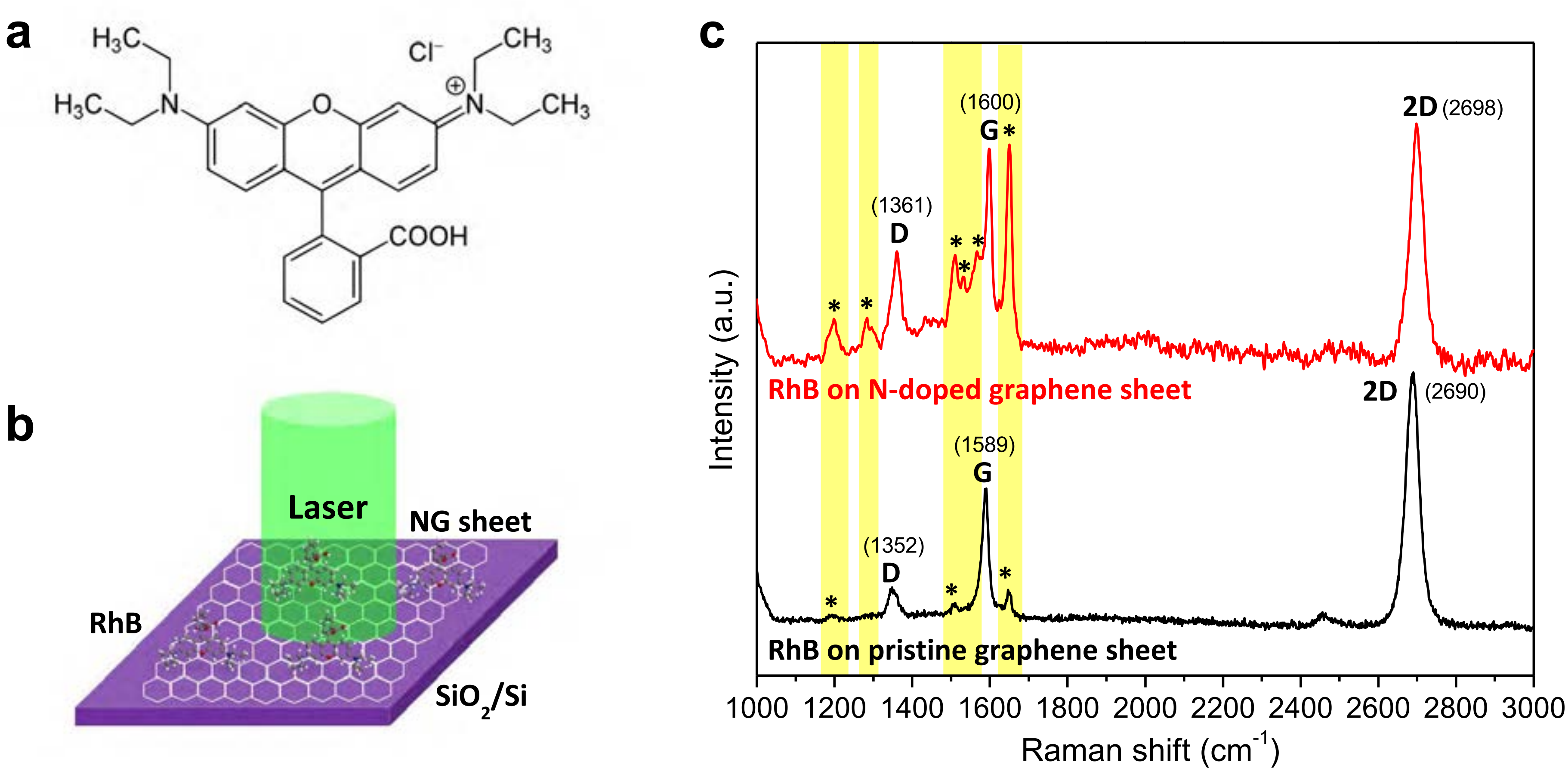
How can we explain the formation of these double N substitutions in Graphene?

What is the driving force?



S. Feng unpublished (2013)

N-doped Graphene: Molecular Sensor



R.T. Lu, et al., Nature Scientific Reports 2, 586 (2012).

Graphene sensing through Raman Spectroscopy

Center for 2-Dimensional and Layered Materials Penn State

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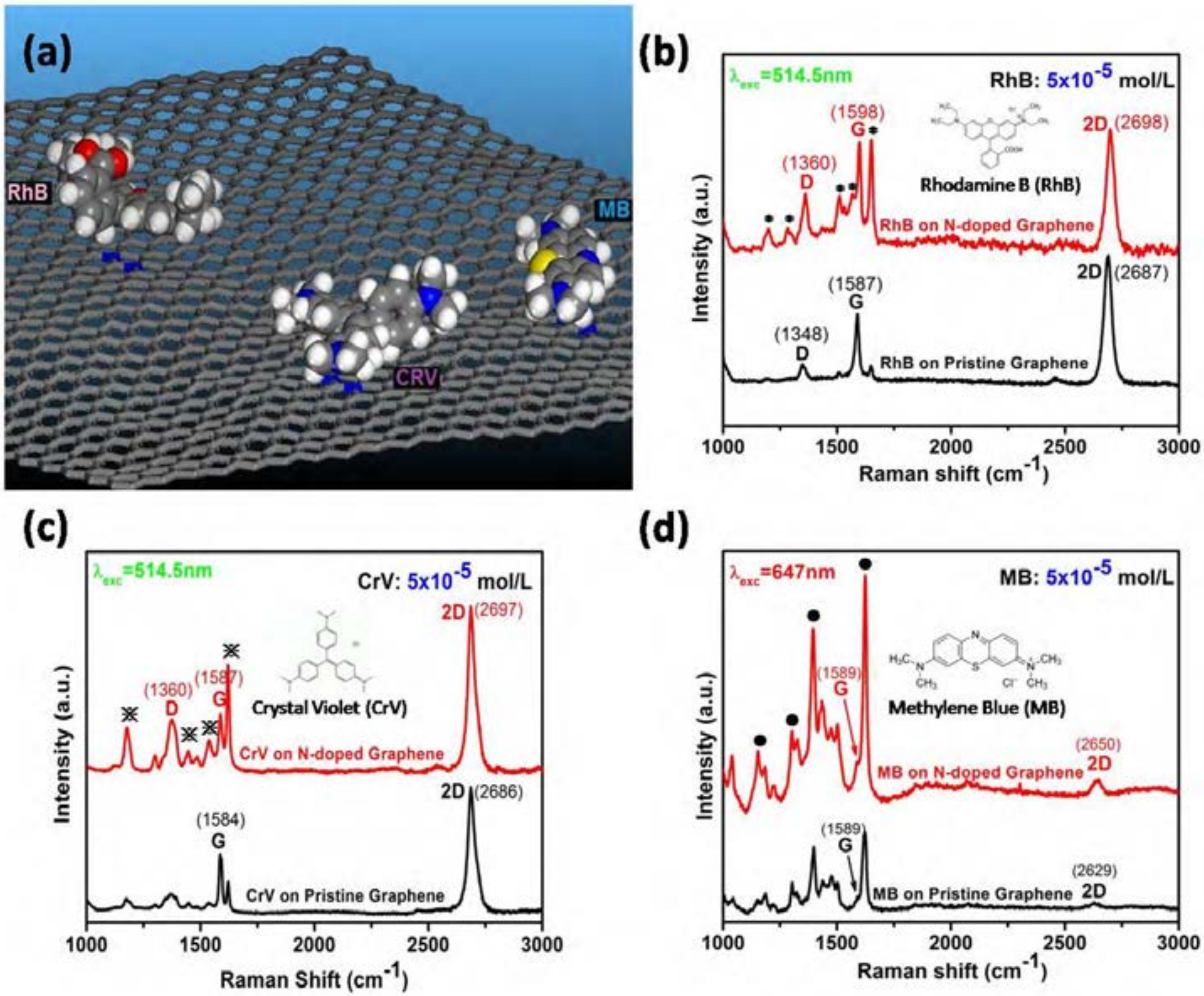
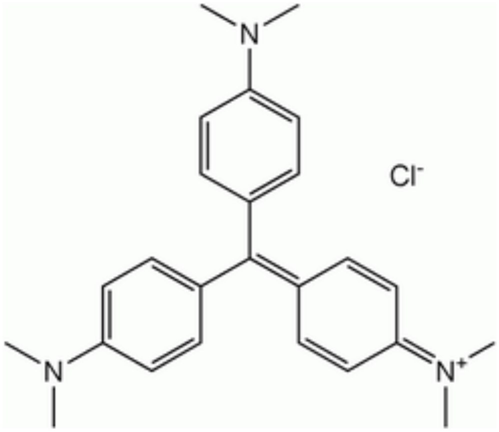
- **Comparison of different dye molecules.**



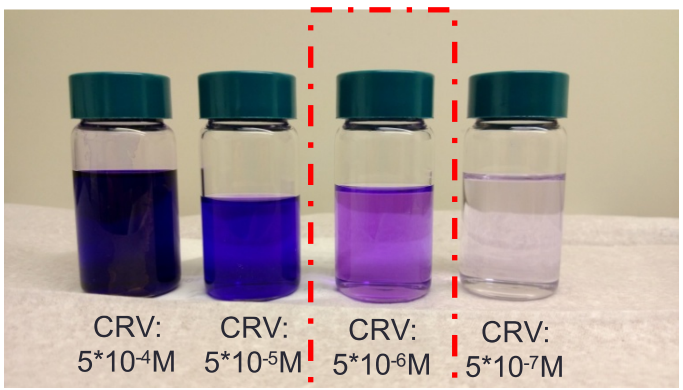
Simin Feng, Maria Cristina Dos Santos, Ruitao Lv, Mauricio Terrones et al., unpublished (2015)

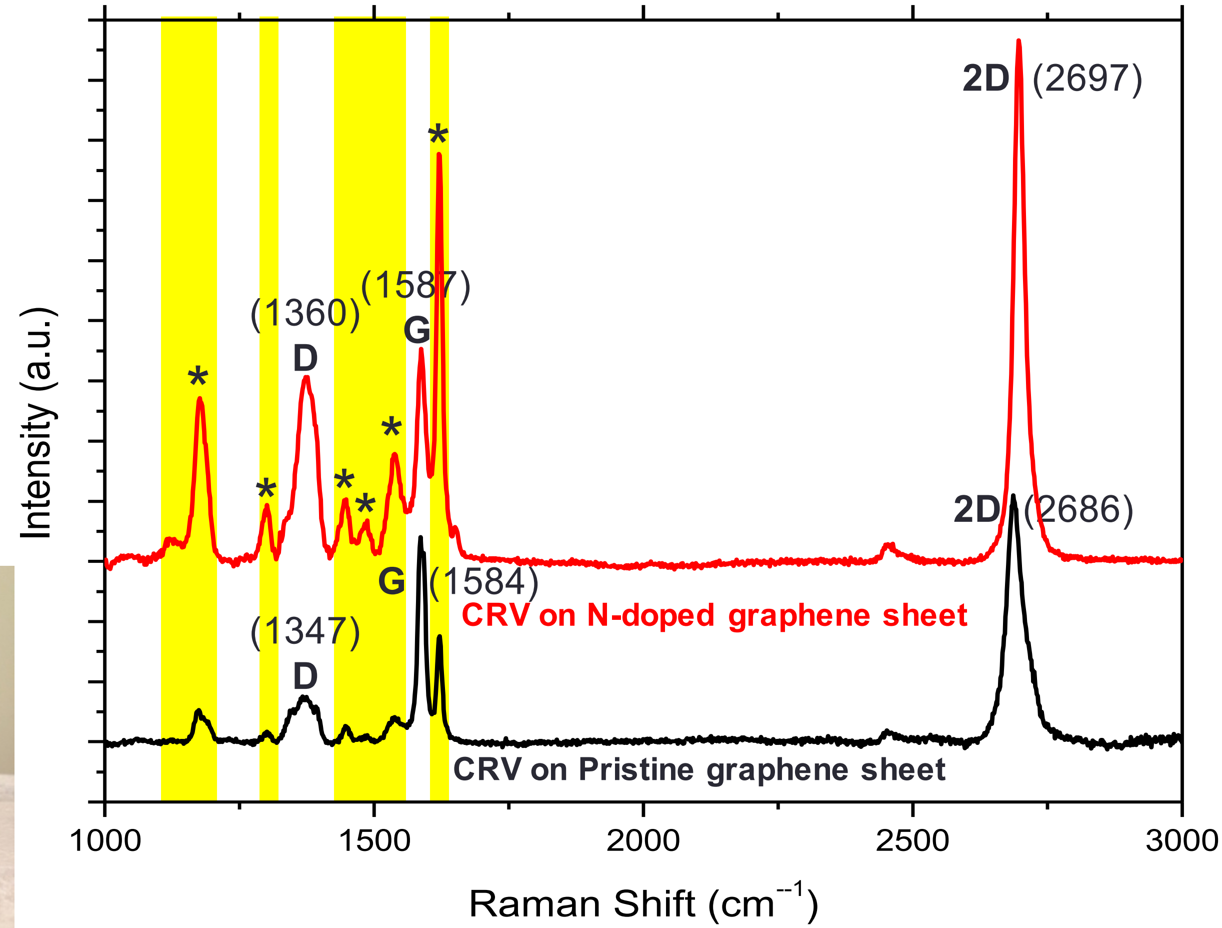
Molecular sensing properties of N-doped graphene

PENNSTATE



Crystal Violet (CRV)





S. Feng unpublished (2013)

Graphene sensing through Raman Spectroscopy

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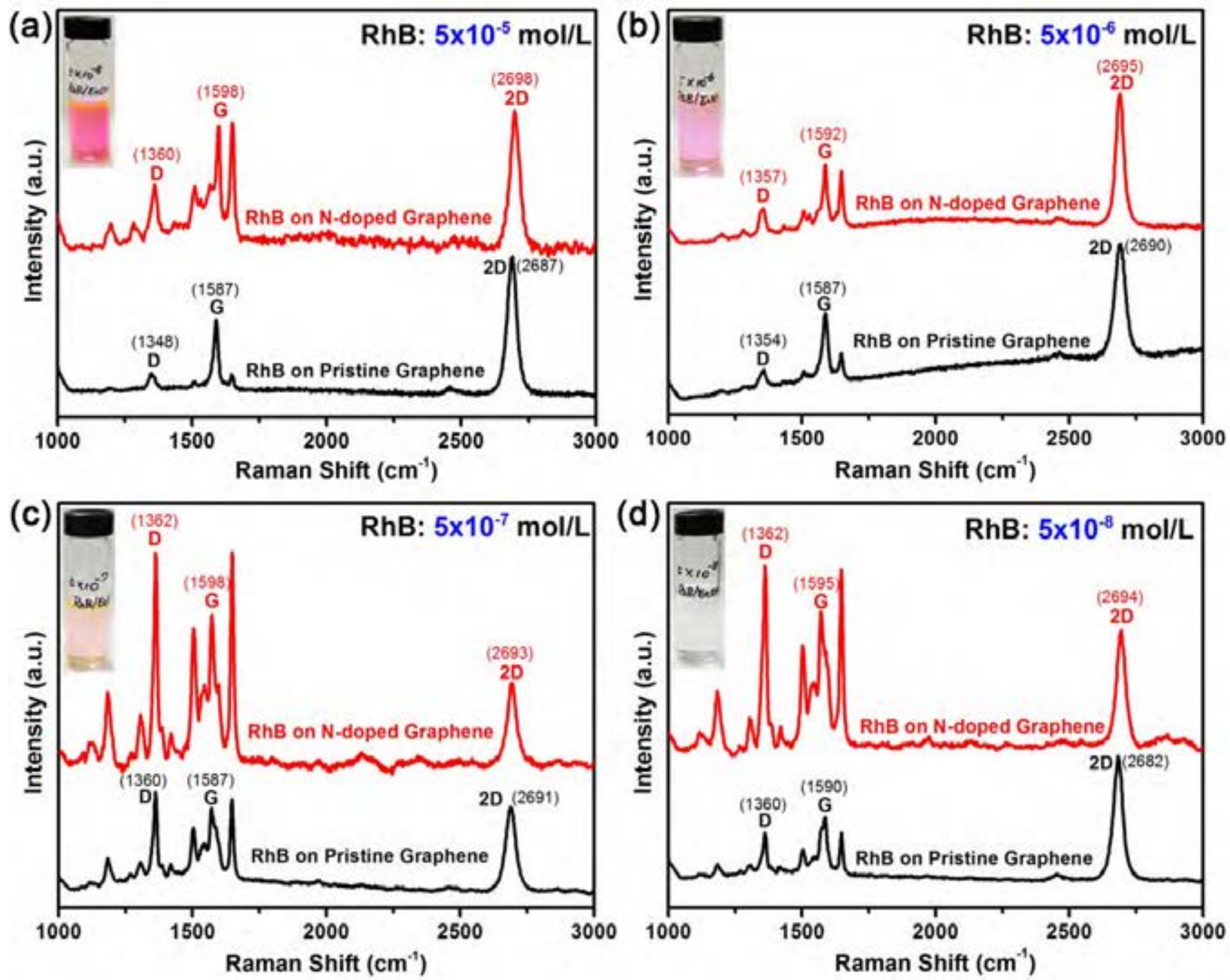
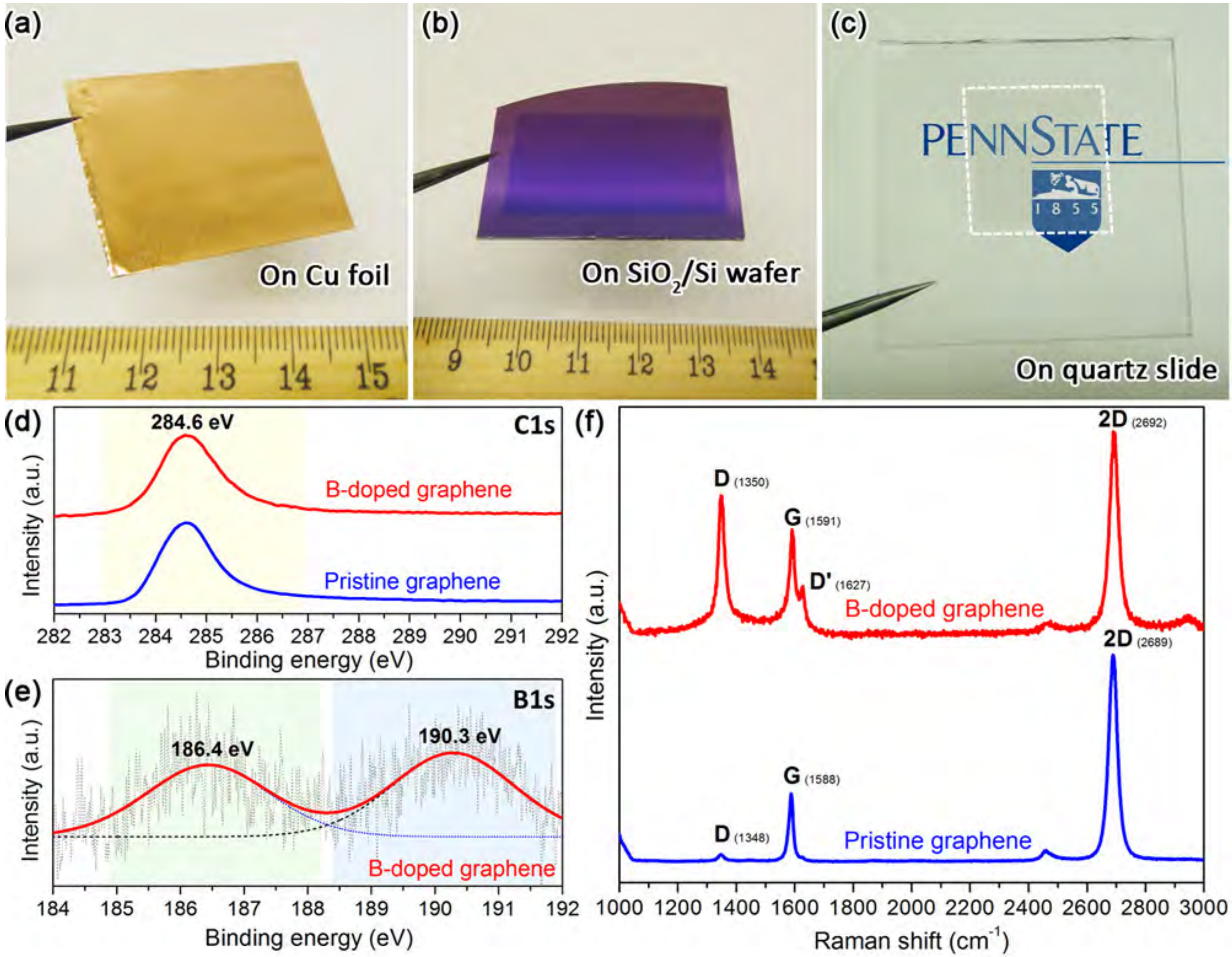
➢ **Comparison of Enhanced Raman scattering effect between NG and PG sheets for probing RhB molecule with different concentration.**



It should be noted here that even with RhB concentration as low as 5 x 10 -8 mol/L, NG sheets can still show very much enhanced Raman signal for different RhB Raman features.

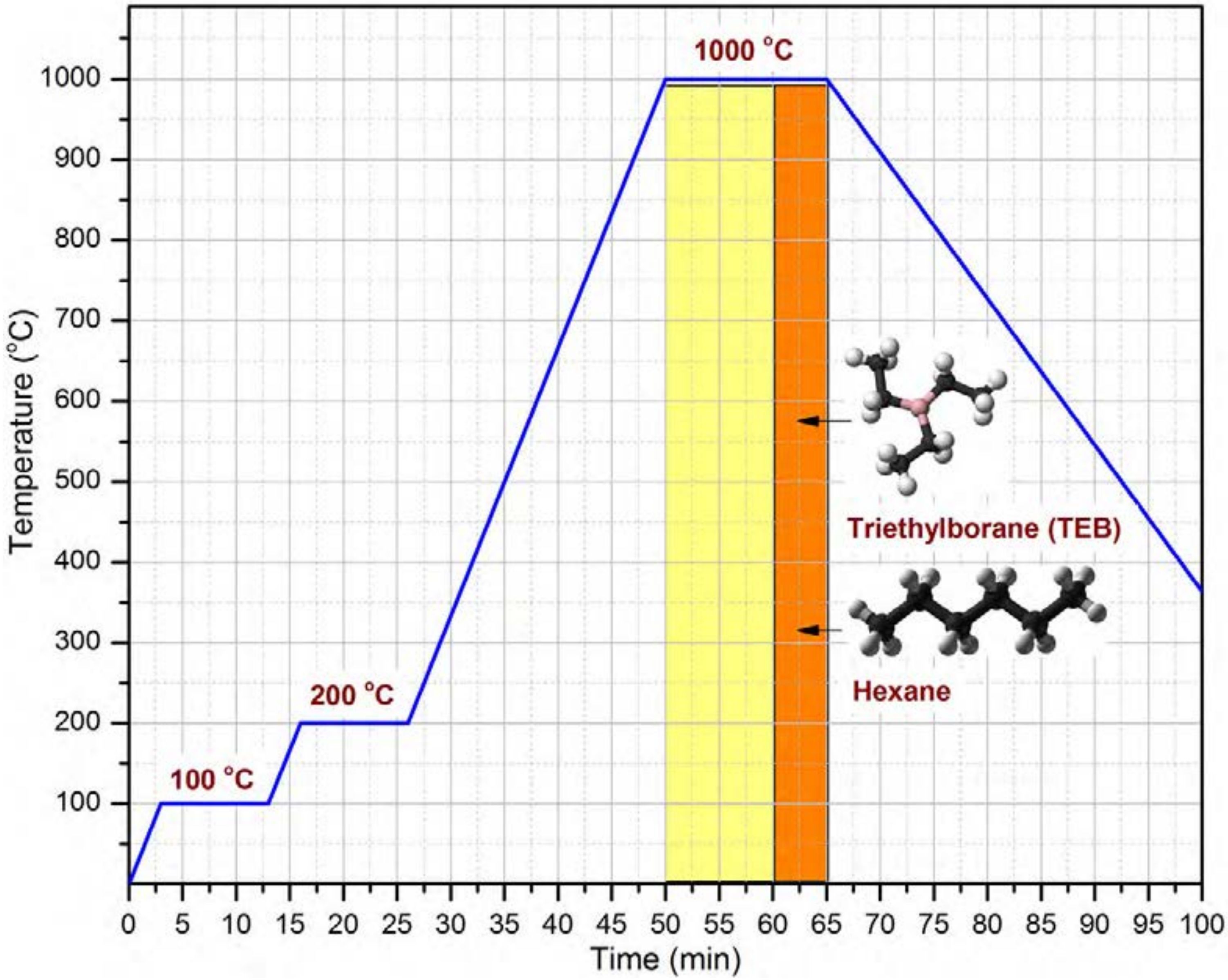
Simin Feng, Maria Cristina Dos Santos, Ruitao Lv, Mauricio Terrones et al., unpublished (2015)

Boron-doped Graphene



R. Lv, et al. *PNAS* ***112****, 14527 (2015)*

Boron-doped Graphene



R. Lv, et al. *PNAS* ***112****, 14527 (2015)*

HTEM / Raman mapping of BG sheet on SiO_2/Si substrate

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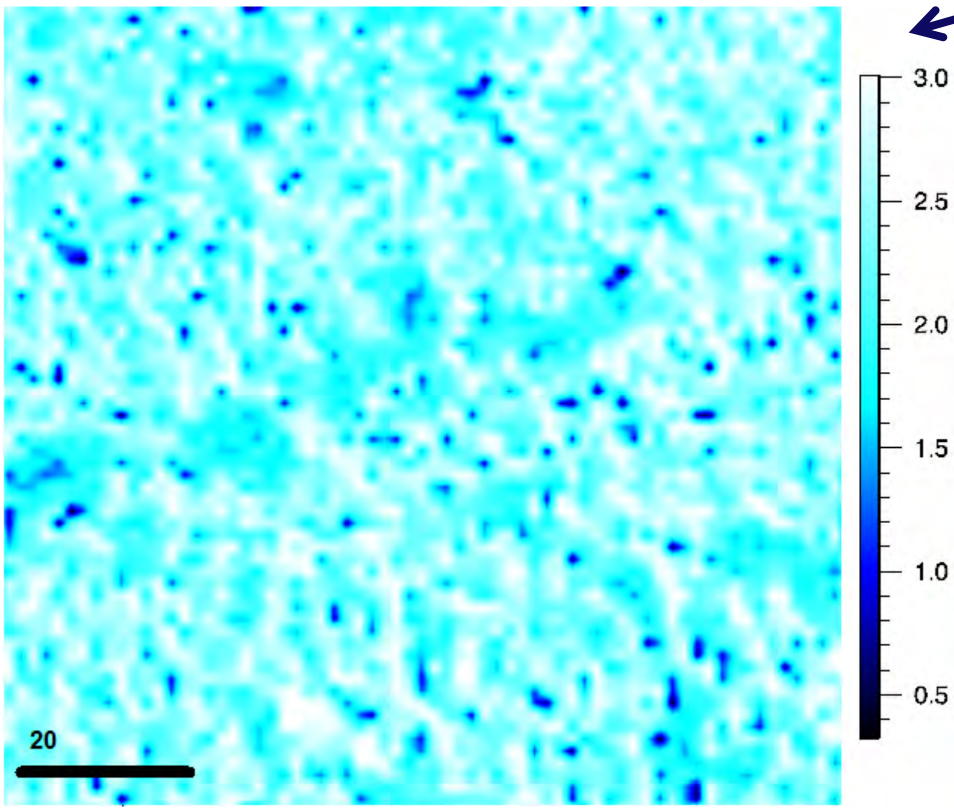
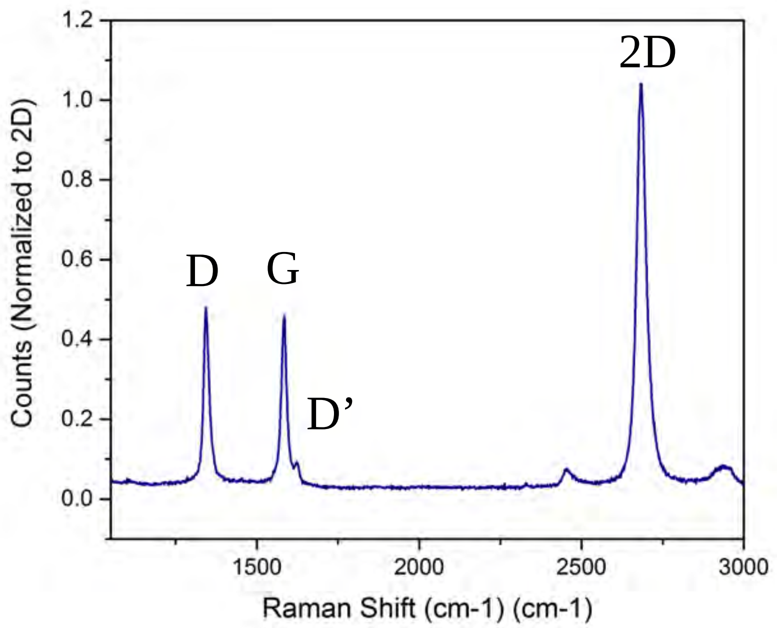


$$\frac{I_{2D}}{I_G}$$



Raman mapping settings:
514 nm, 4.8 mW, 2 s, 100x, Spot size ≈ 1 µm, Area:47 x 44.5 μm^2, Raster scan, Step: 0.4 µm, Total 13,216 points,Time ≈ 18 hours

R. Lv, et al. *PNAS **112**, 14527 (2015)*

STM / STS of BG sheet on SiO_2/Si substrate

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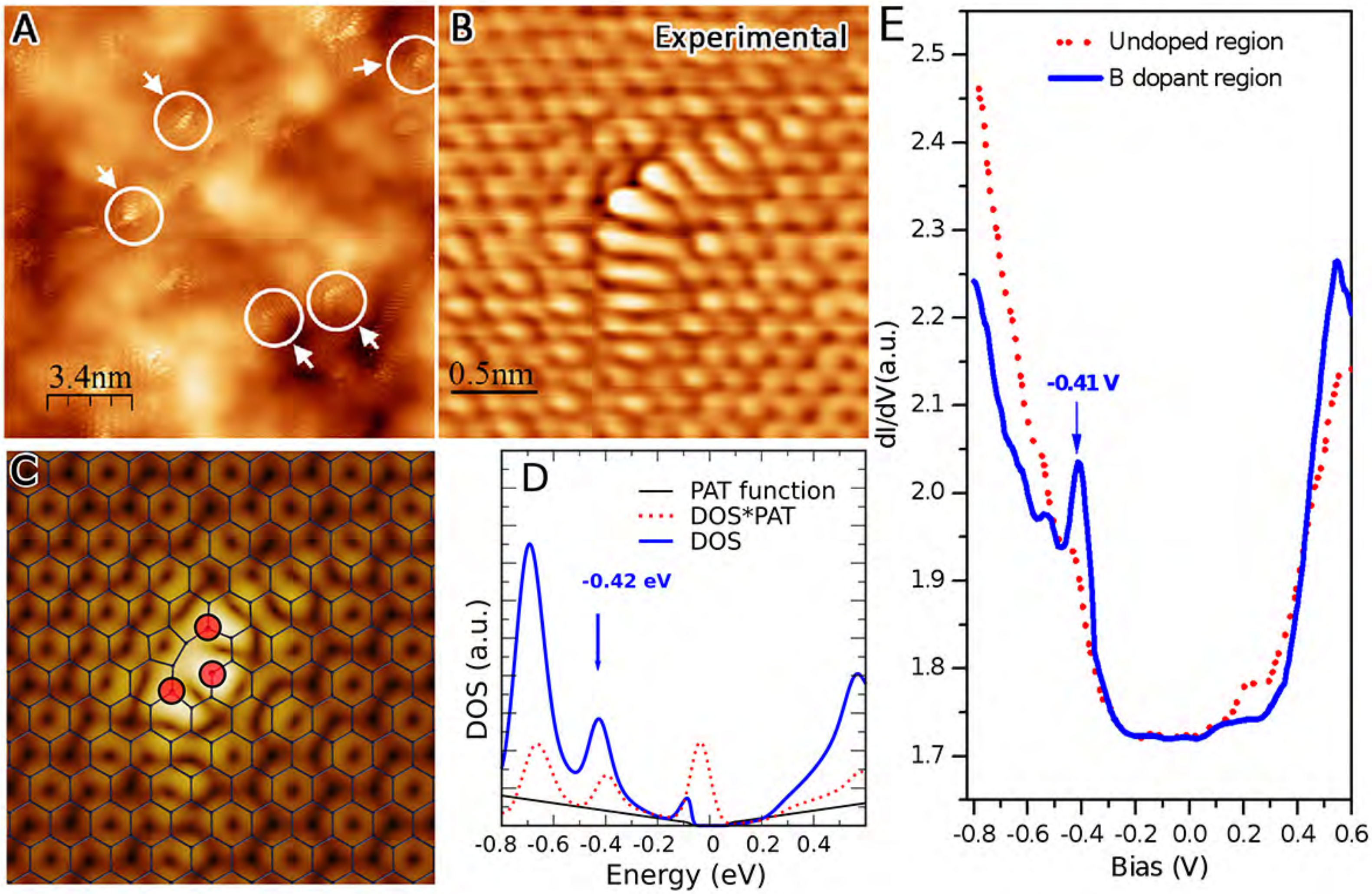

with M.G. Pan (ORNL), V. Meunier (RPI) & A. Botello & J.C. Charlier (UCL)

R. Lv, et al. *PNAS* ***112****, 14527 (2015)*

B-doped Graphene as Gas sensors: NO_2 and NH_3

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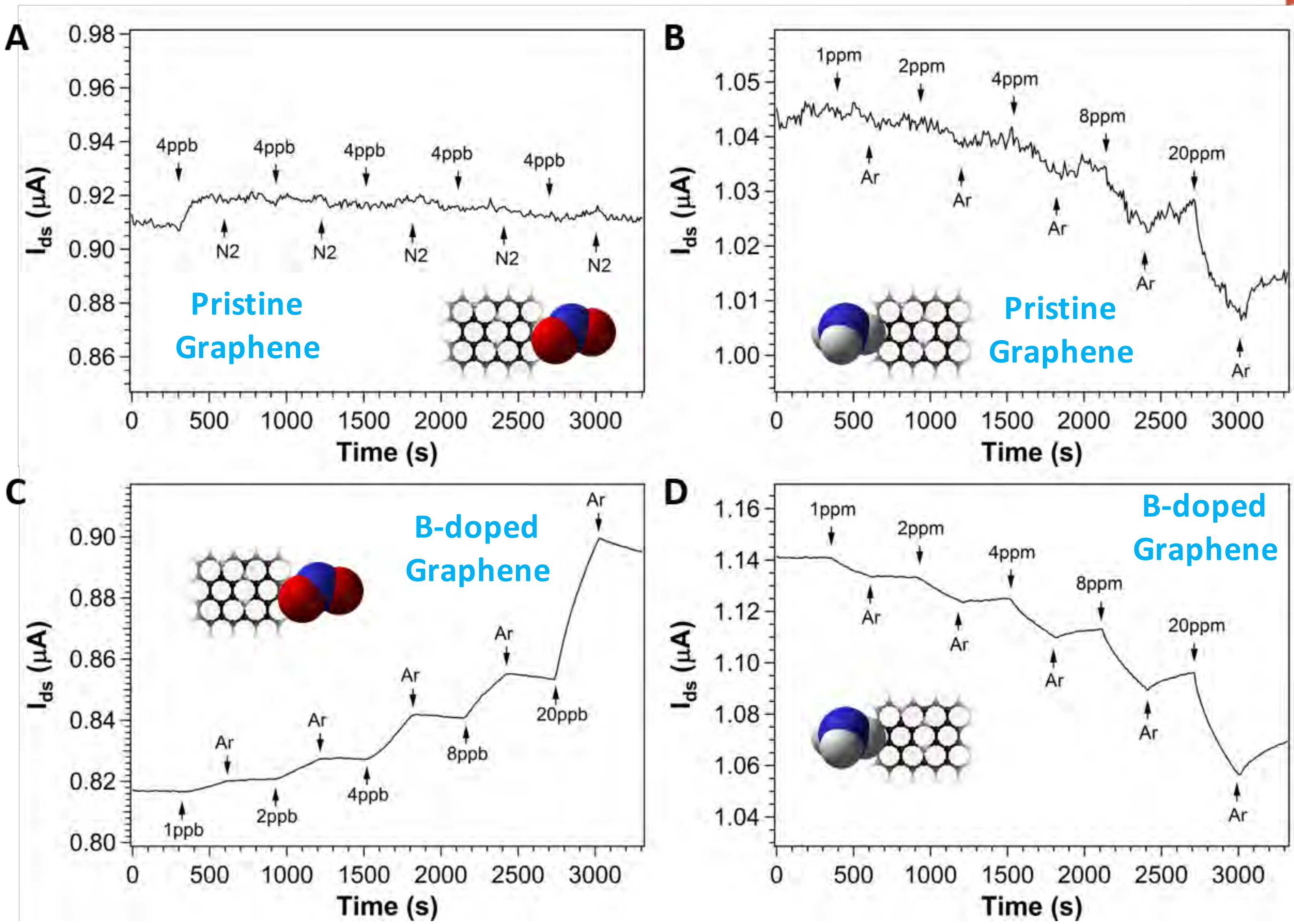

In collaboration with G. Chen and A. Harutyunyan

R. Lv, et al. *PNAS* ***112****, 14527 (2015)*

B-doped Graphene as Gas sensors: NO_2 and NH_3

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Target gas	Sensing material	Lowest concentration tested	Detection limit
NO_2	Mechanically exfoliated graphene(47)	100 ppm	--
	CVD graphene-like films(48)	65 ppm	--
	Ozone-trated graphene(49)	200 ppm	1.3 ppb
	Ethylenediamine-modified rGO(50)	1 ppm	70 ppb
	Sulfonated rGO(50)	5 ppm	3.6 ppm
	Epitaxial graphene from SiC(51)	2.5 ppm	--
	MPECVD graphene(52)	100 ppm	--
	rGO(53)	5 ppm	--
	rGO(54)	2 ppm	--
	Carbon Nanotubes/rGO hybrid(55)	0.5 ppm	--
	Mechanically exfoliated graphene(56)	1 ppm	The order of 1 ppb
	CVD graphene(57)	100 ppb	100 ppb
NH_3	rGO(53)	5 ppm	--
	Mechanically exfoliated graphene(56)	1 ppm	--
	CVD graphene(58)	65 ppm	--
	rGO/Polyaniline hybrid(59)	5 ppm	--
	Mechanically exfoliated graphene(60)	10 ppm	--
	rGO(61)	20 ppm	--
	CVD graphene(57)	500 ppb	500 ppb
	rGO(62)	10000 ppm (1%)	--
	rGO(54)	10000 ppm (1%)	--

R. Lv, et al. *PNAS* ***112****, 14527 (2015)*

Si-doped Graphene: Synthesis

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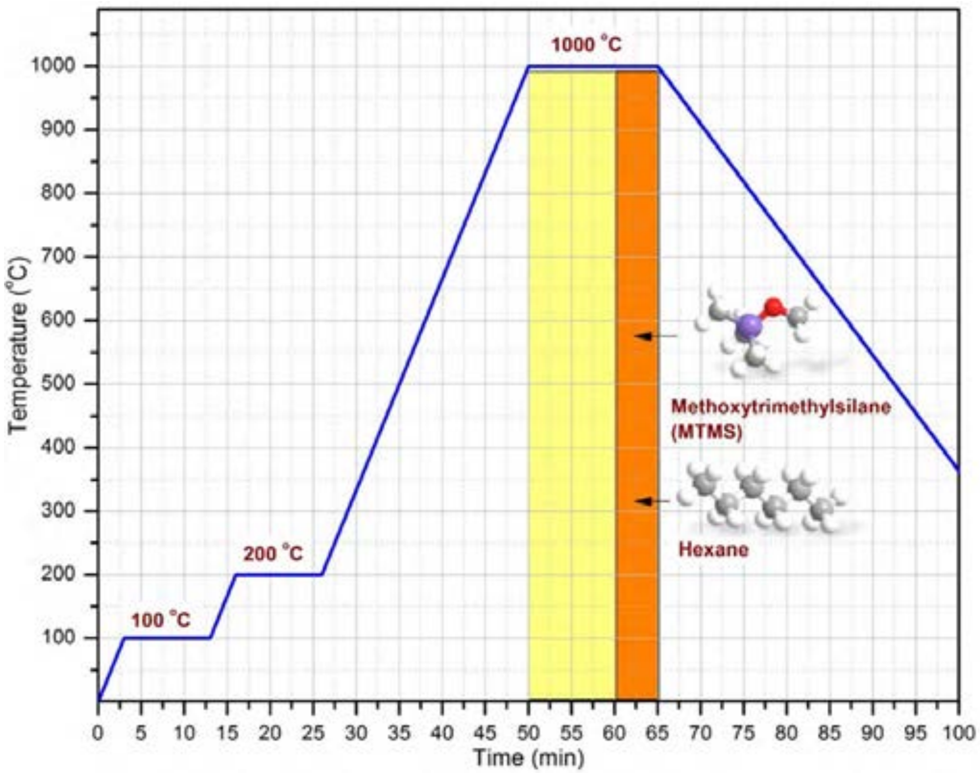

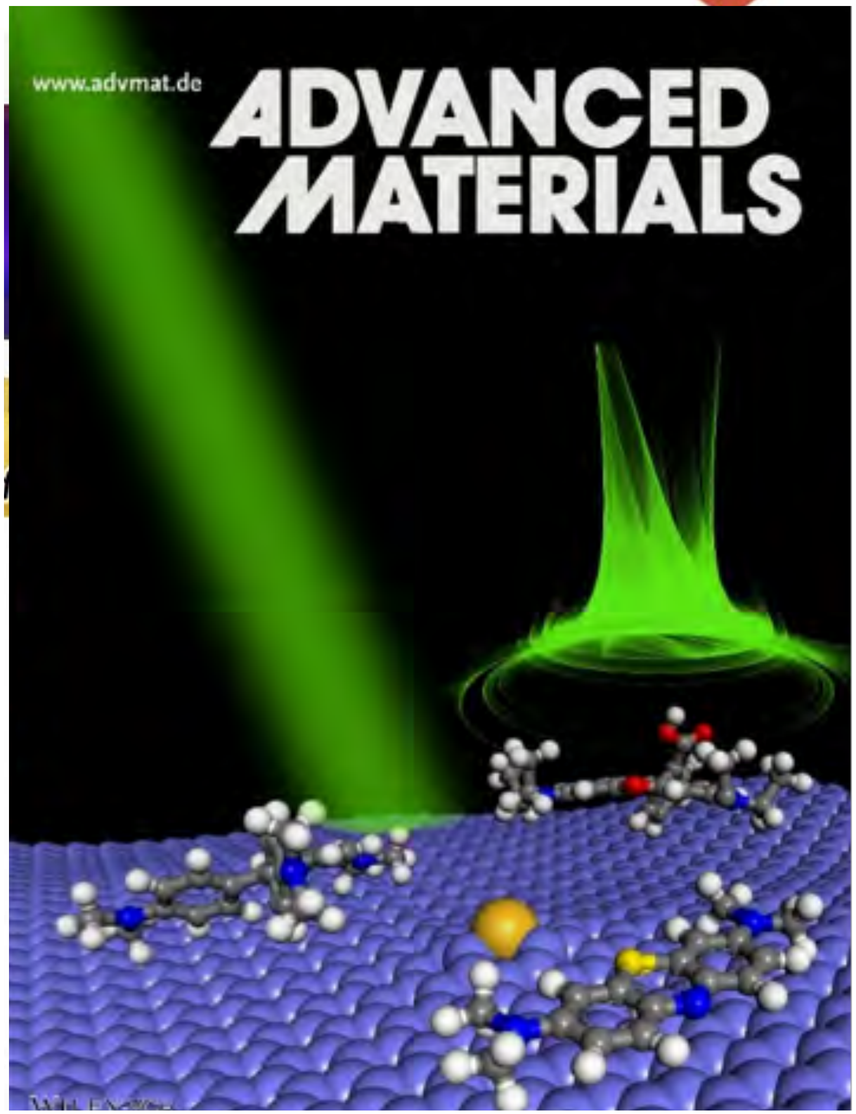

R.T. Lu, et al., Advanced Materials (2014)

Si-doped Graphene: Raman spectroscopy & XPS analysis

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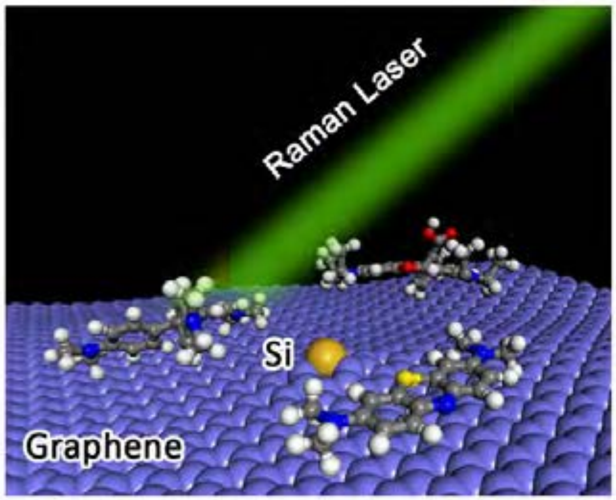
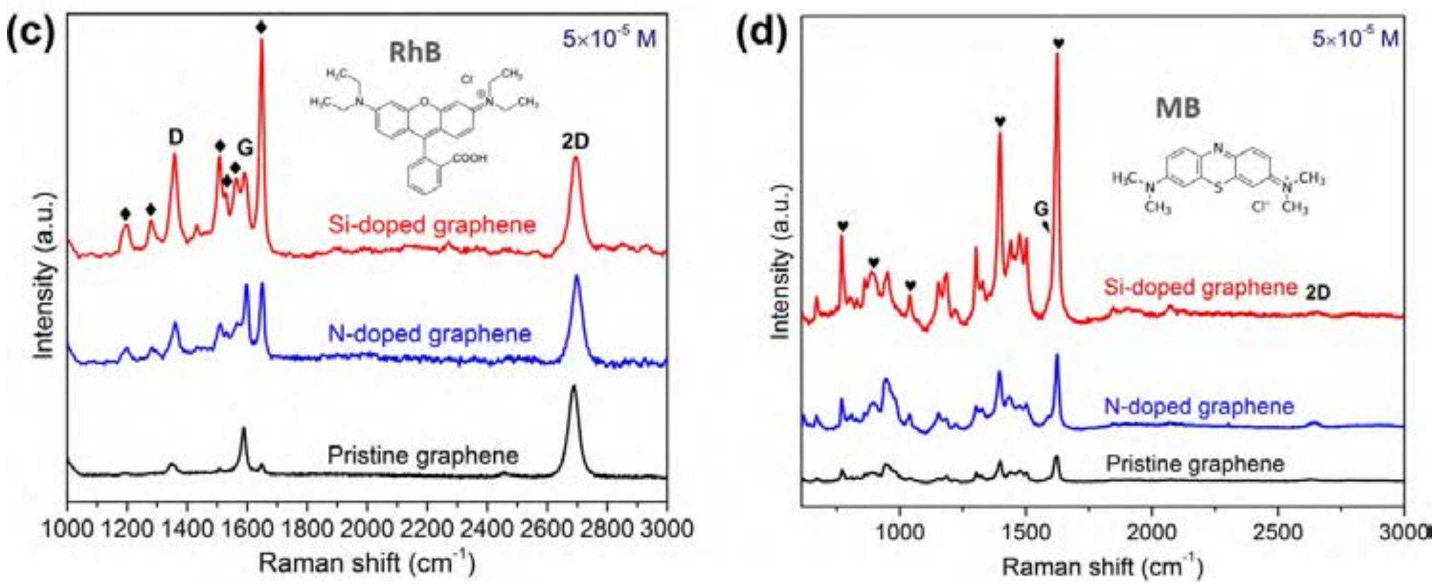


- **Challenges remaining**

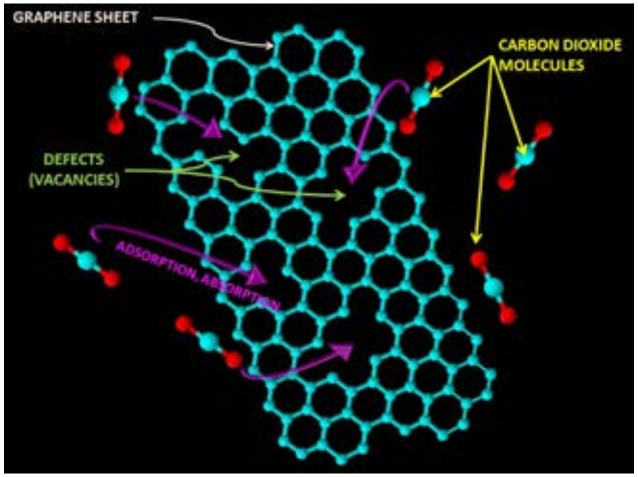
Need to image Si in graphene by STM or HRTEM

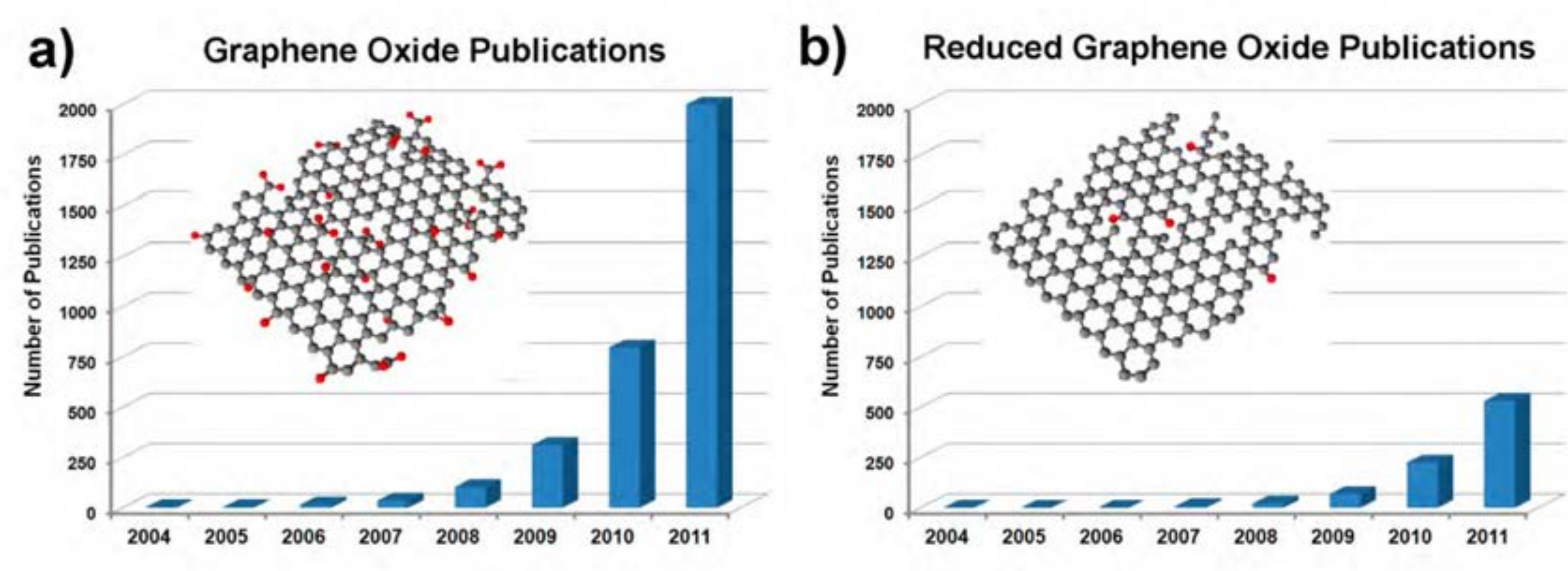
Is there a preferential location(s) for Si within the graphene lattice?



R.T. Lu, et al., Advanced Materials (2014)

Graphene Oxide (GO) and Reduced GO





Varela-Rizo, H., Martin-Gullon, I, Terrones, M. ***ACS Nano (2012)***

Dünnste Kohlenstoff-Folien

H.P. Boehm, A. Clauss, G.O. Fischer and U. Hofmann

[Z. Naturforschung 17b, 150 (1962)]

Bei der Reduktion von Graphitoxyd in sehr verdünnter alkalischer Suspension entsteht extrem feinlamellarer Kohlenstoff. Die Bestimmung der Dicke der dünnsten Lamellen aus dem Kontrast im Elektronenmikroskop ergab, daß sie nur aus einigen wenigen, z. T. wahrscheinlich nur aus einer einzigen Kohlenstoff-Sechseckschicht des Graphitgitters bestehen. Das Ergebnis wird gestützt durch röntgenographische Untersuchungen sowie durch Messungen der spezifischen Oberfläche.

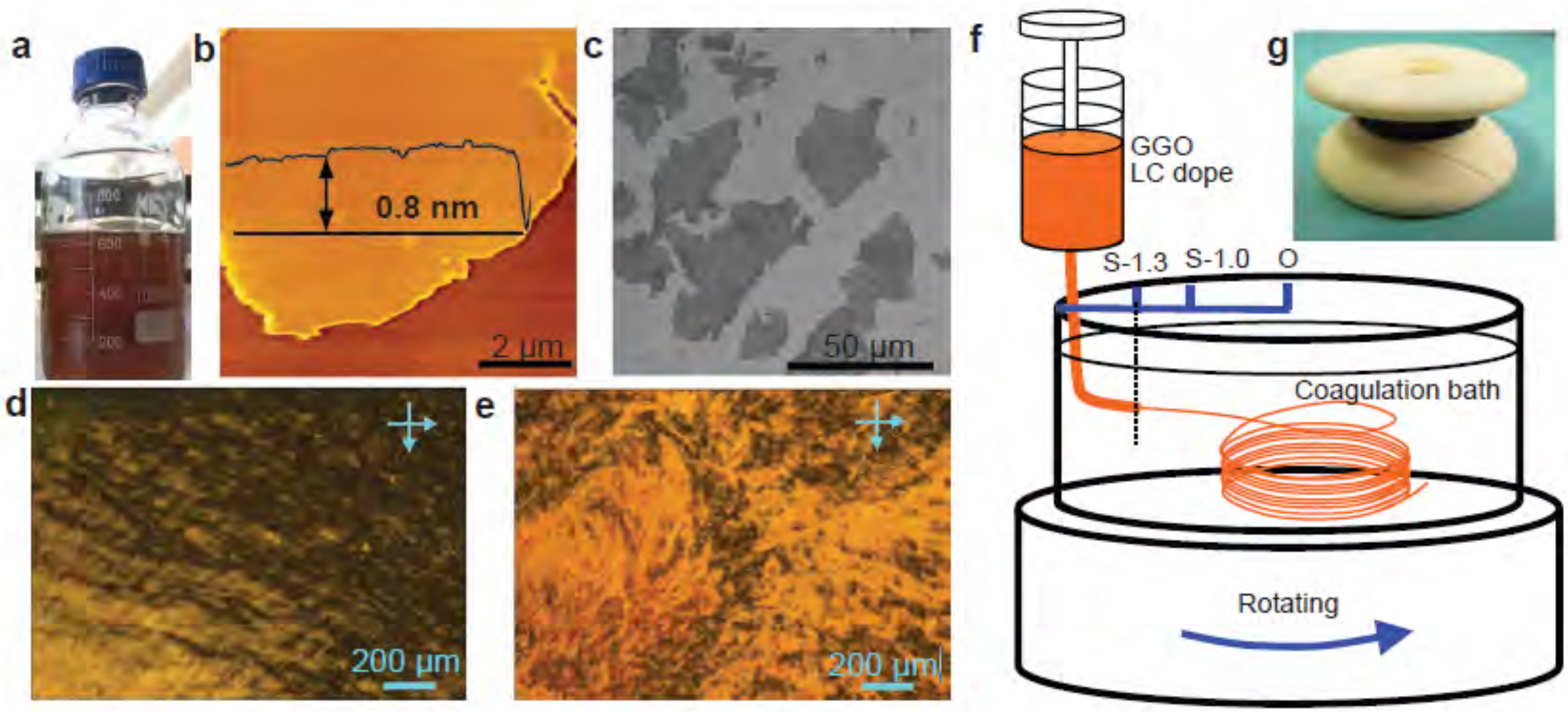
The thinnest carbon sheets

The reduction of graphite oxide in a very dilute alkaline suspension produced extremely thin carbon lamellae. An estimation of the thickness of the thinnest lamellae from TEM contrast showed that they consisted of very few carbon layers, **probably a single one**. This result was supported by X-ray studies as well as by measurements of specific surface area.

Courtesy of Peter Thrower

GO fibers by wet-spinning

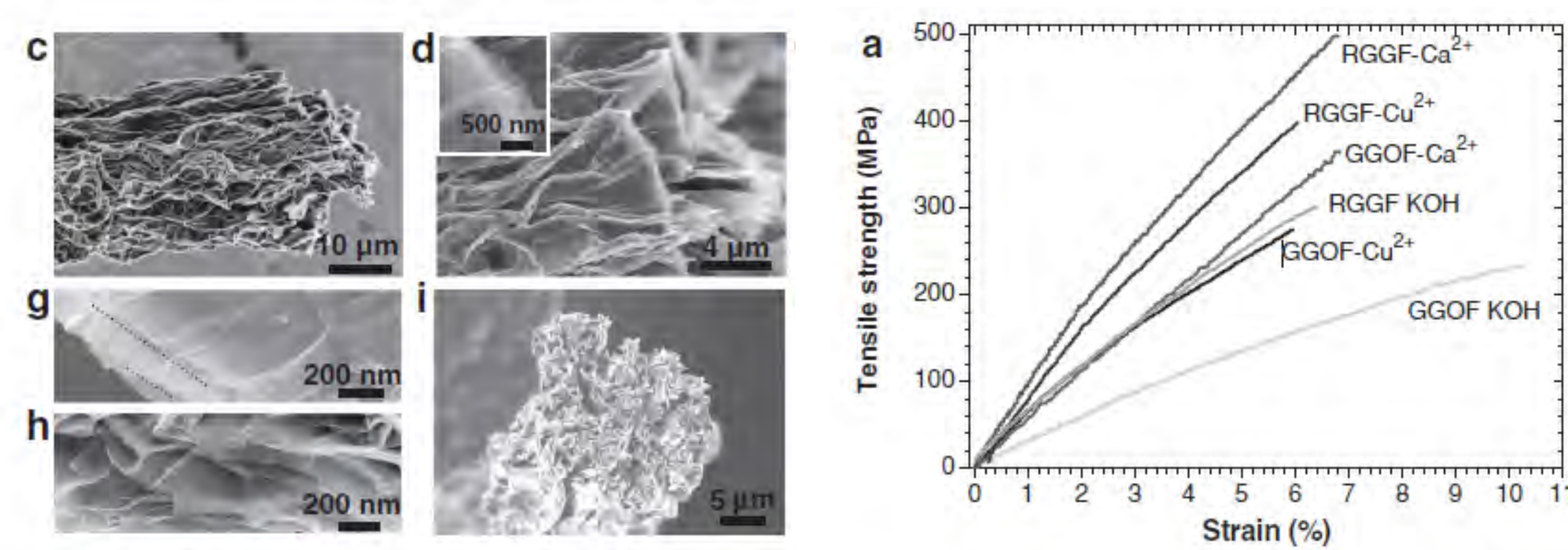
- Preparation of GO dispersion.
- Use the colloidal instability of GO to make a fiber



Xu *et al. Adv. Mater.* **2013**, *25*, 188

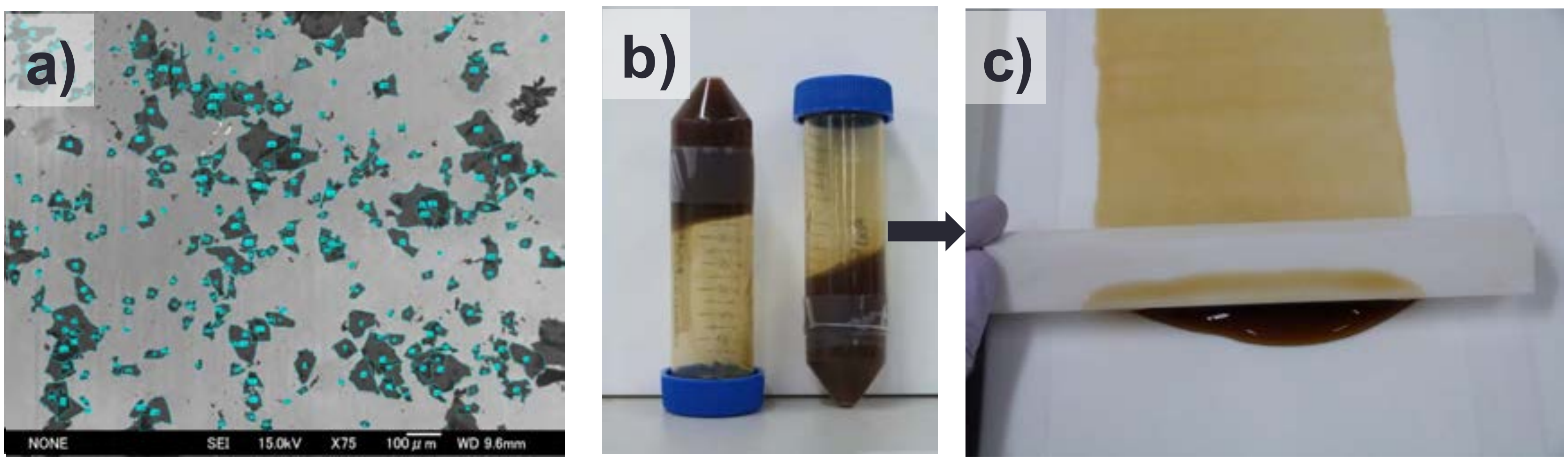
GO fibers by wet-spinning

- Preparation of GO dispersion.
- Injection of GO dispersion in a coagulation bath.
- Drying and reduction to graphene.



Xu *et al. Adv. Mater.* **2013**, *25*, 188

Film preparation by bar-coating



Average size=2200 μm^2

In collaboration with M. Endo

R. Cruz-Silva, et al. ACS Nano 8, 5959-5967 (2014)

Free standing GO films by casting

R. Cruz-Silva, et al. ACS Nano 8, 5959-5967 (2014)

Free standing GO films by casting

Large area free-standing graphite oxide film lifting

- Film prepared by bar coating a 0.7 mg/ml graphite oxide dispersion and drying at room temperature.
- Film total mass 279 mg, total area 792 cm^2, average surface density= 0.35 mg/cm^2.

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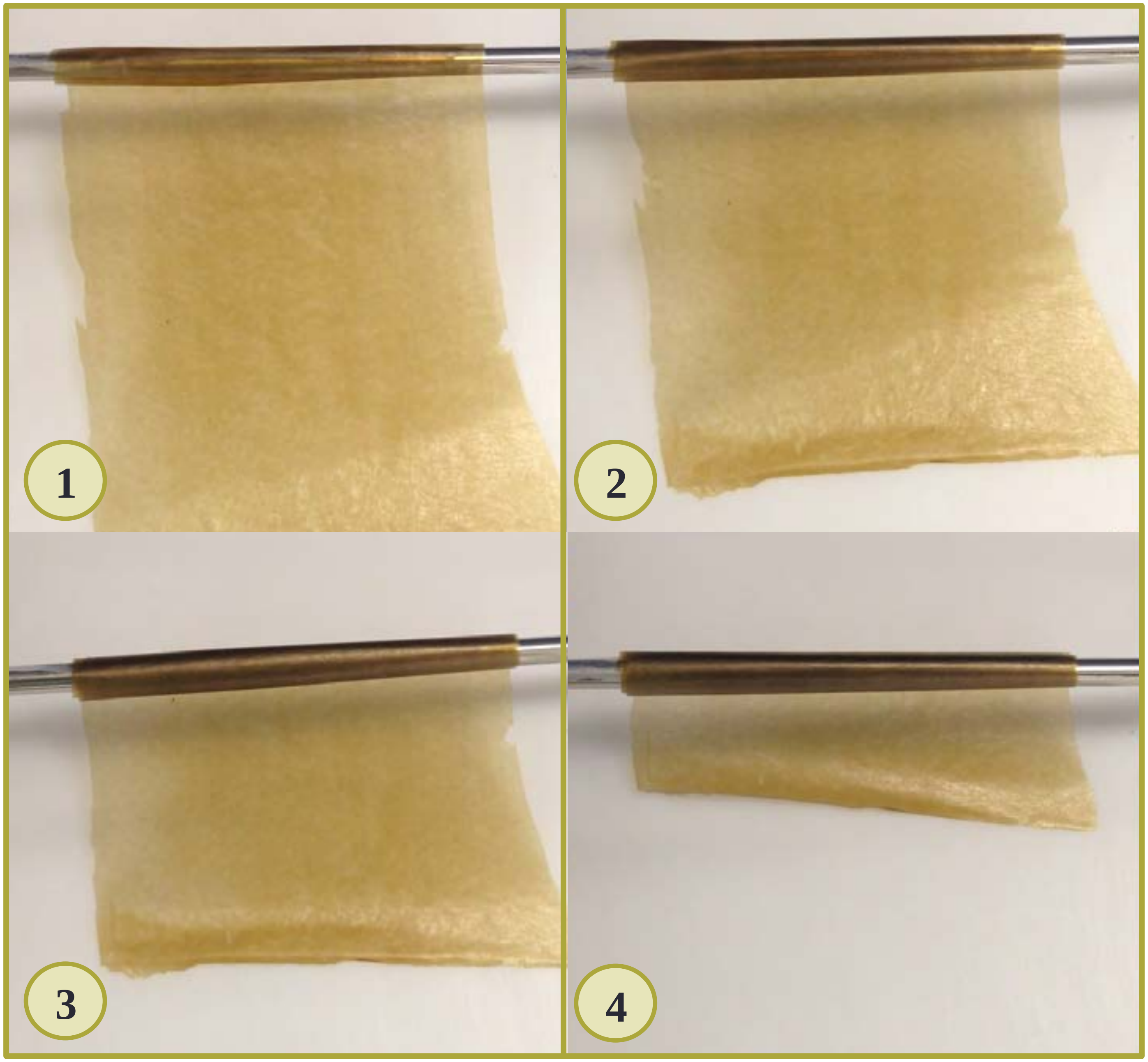
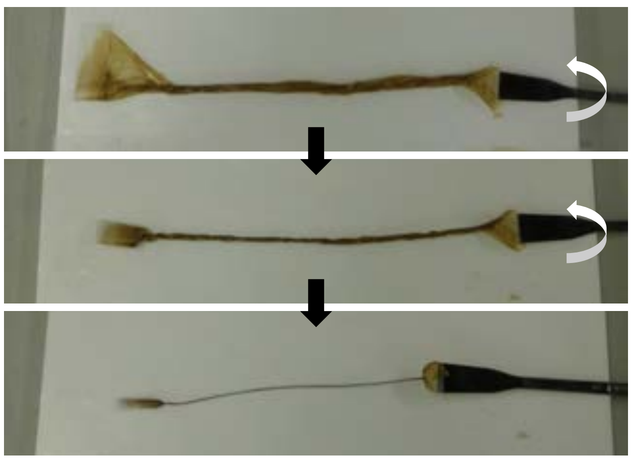
R. Cruz-Silva, et al. ACS Nano 8, 5959-5967 (2014)

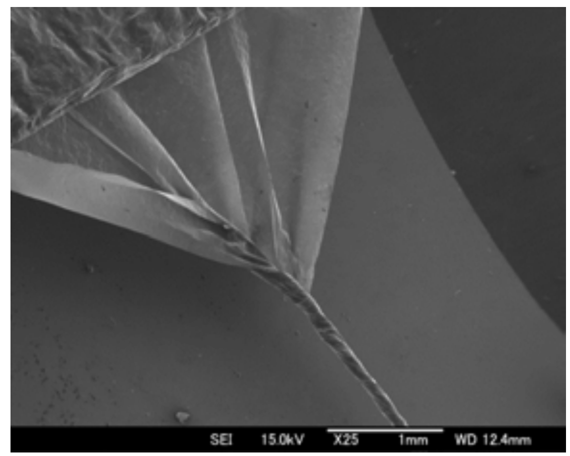
Scalability Tests: GO Films



Making a GO fiber from a film.

- Twisting
- Simple method.
- Solvent-free





1 mm

R. Cruz-Silva, et al. ACS Nano 8, 5959-5967 (2014)

Making a GO fiber from a film.

Transformation of graphite oxide film into a fiber by scrolling.

- Graphite oxide film with density 0.6 mg/cm^2 was scrolled into a fiber.

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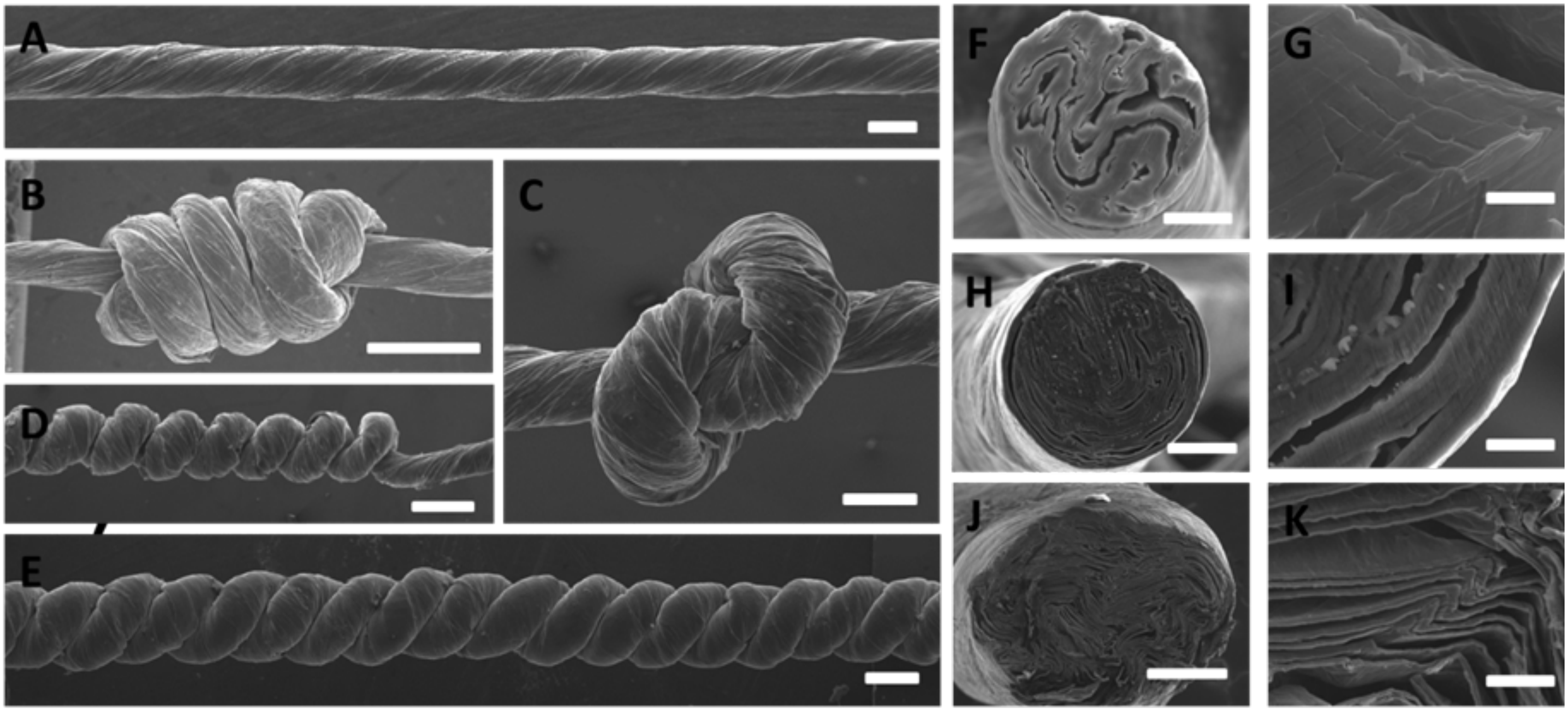
R. Cruz-Silva, et al. ACS Nano 8, 5959-5967 (2014)

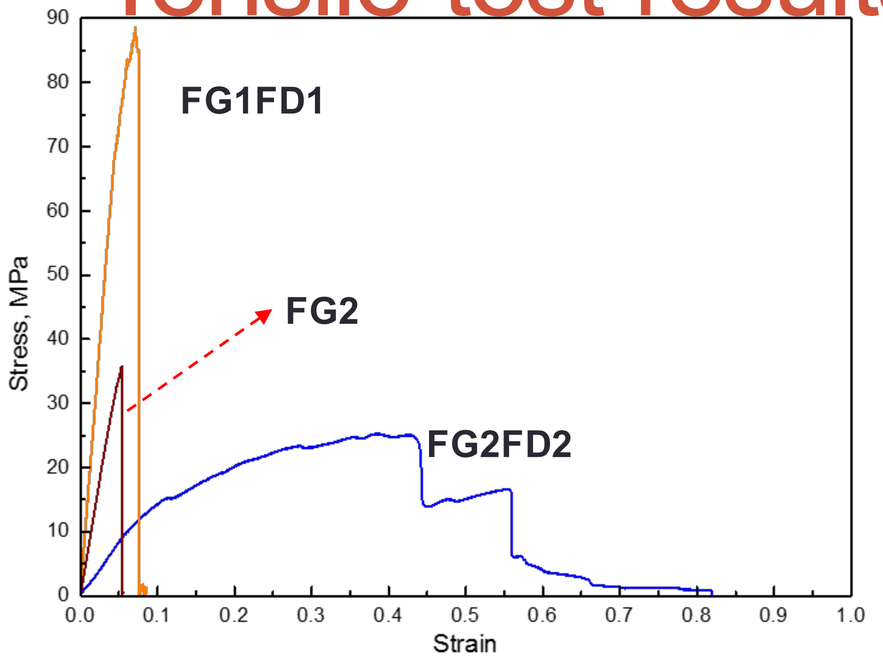
Morphology of GO fibers.



In collaboration with M. Endo

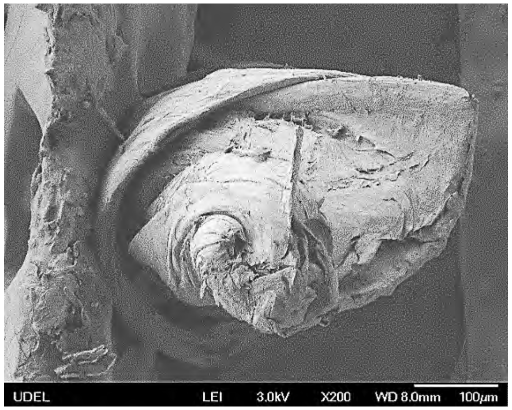
R. Cruz-Silva, et al. ACS Nano 8, 5959-5967 (2014)

Tensile test results: diameter effect



FG1FD1

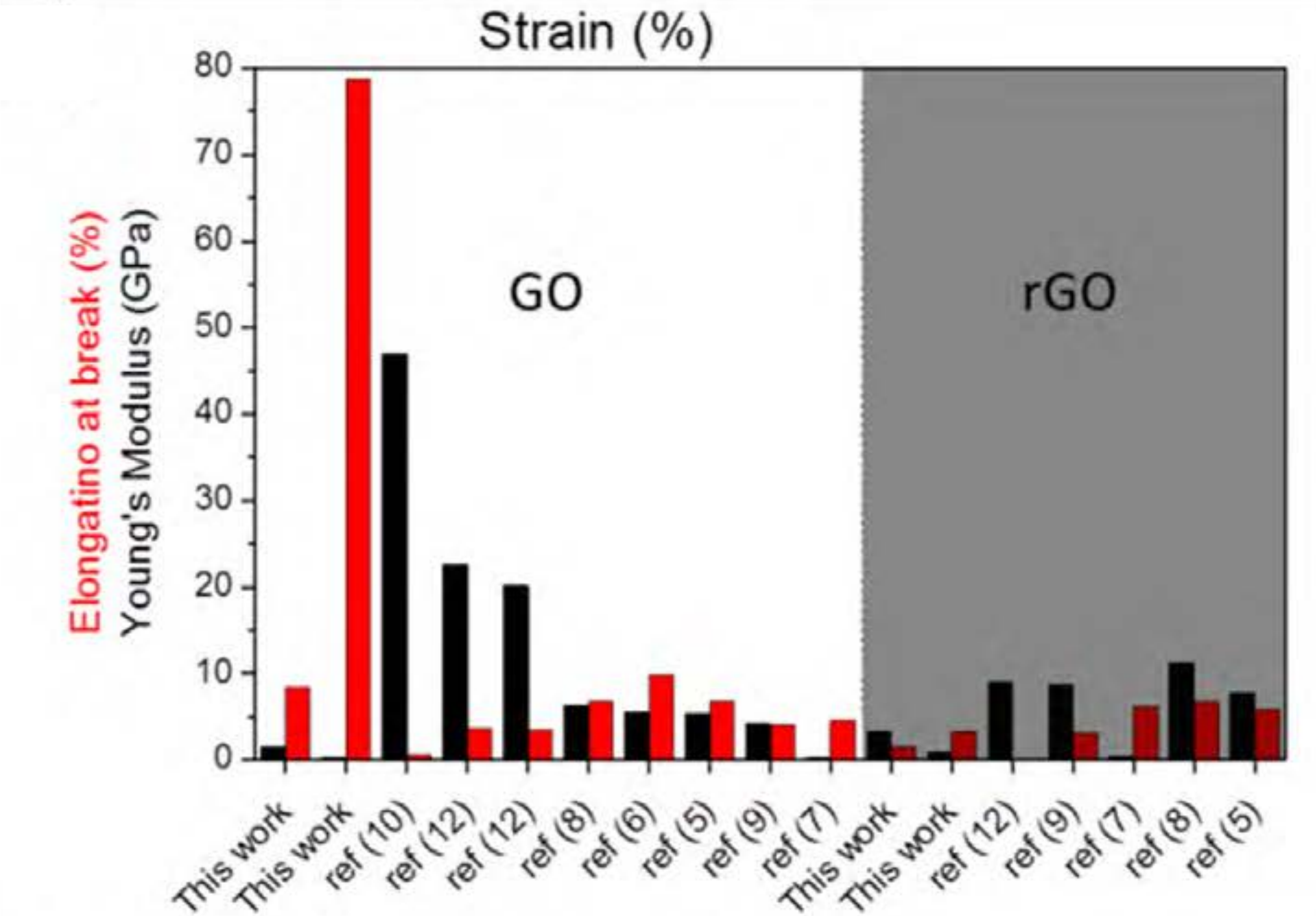
FG2FD2



R. Cruz-Silva, et al. Submitted (2013)

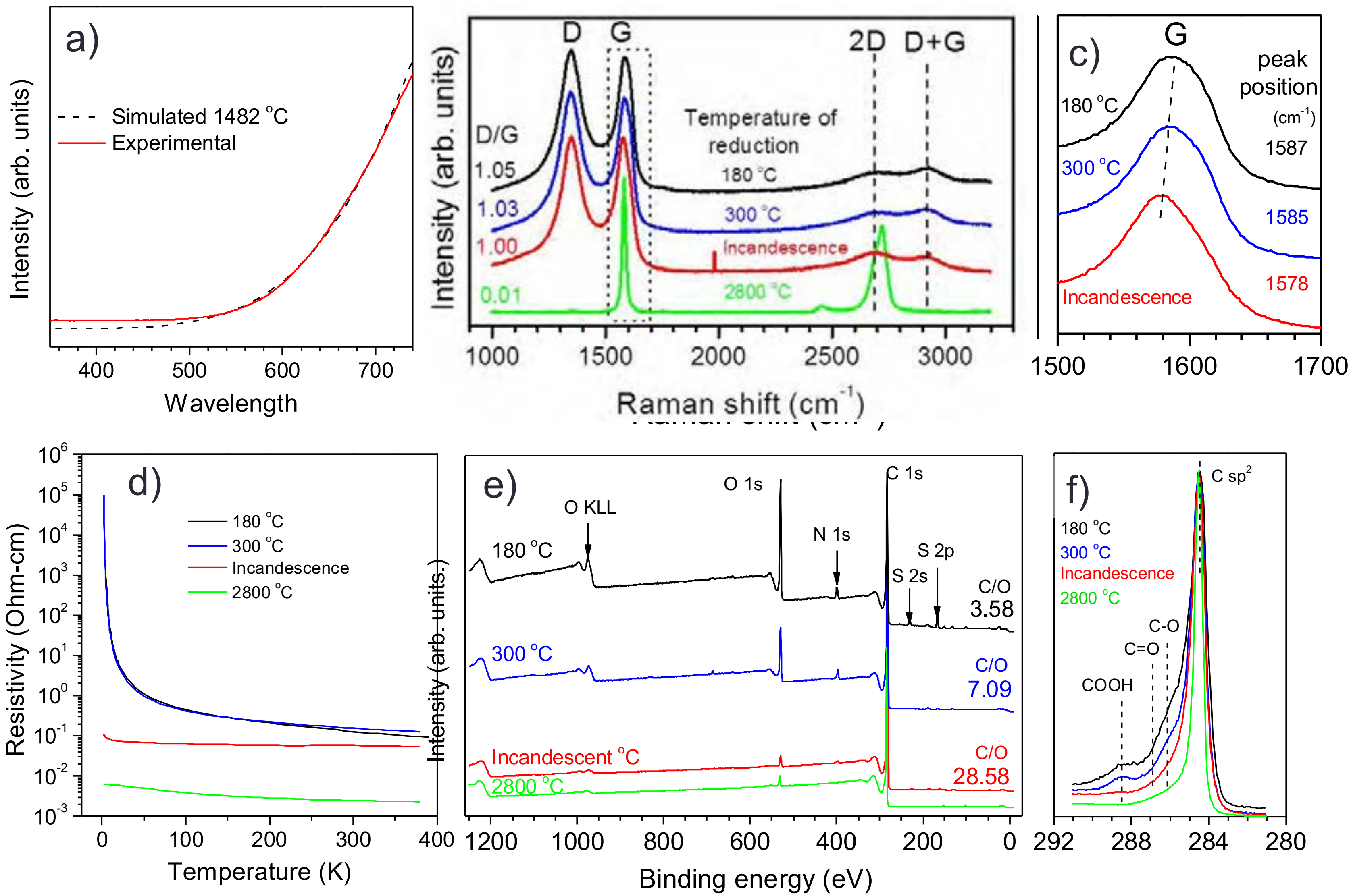
	Young's Modulus, MPa		Tensile Strength, MPa		Toughness, MPa		Elongation at Break, %	
	AVE	STDEV	**AVE**	STDEV	**AVE**	STDEV	**AVE**	STDEV
FG1FD1 (Fiber ; D=100um)	**1,584**	98.8	**85.9**	11.20	**4.31**	1.68	**8.30**	2.26
FG2 (Film ; A=7 mmX5.8 um =40,600um2)	**792**	87.0	**36.1**	0.35	**1.06**	0.06	**5.37**	0.03
FG2FD2 (Fiber ; D=300um A (including air space)=70,650um2)	**186**	17.6	**22.5**	6.04	**10.52**	1.12	**70.48**	18.05
FG2FD2 estimated (Fiber ; A (w/o air space)=40,600um^2)	**324**	30.6	**39.2**	10.51	**18.30**	1.95	**70.48**	18.05

Tensile test results: diameter effect



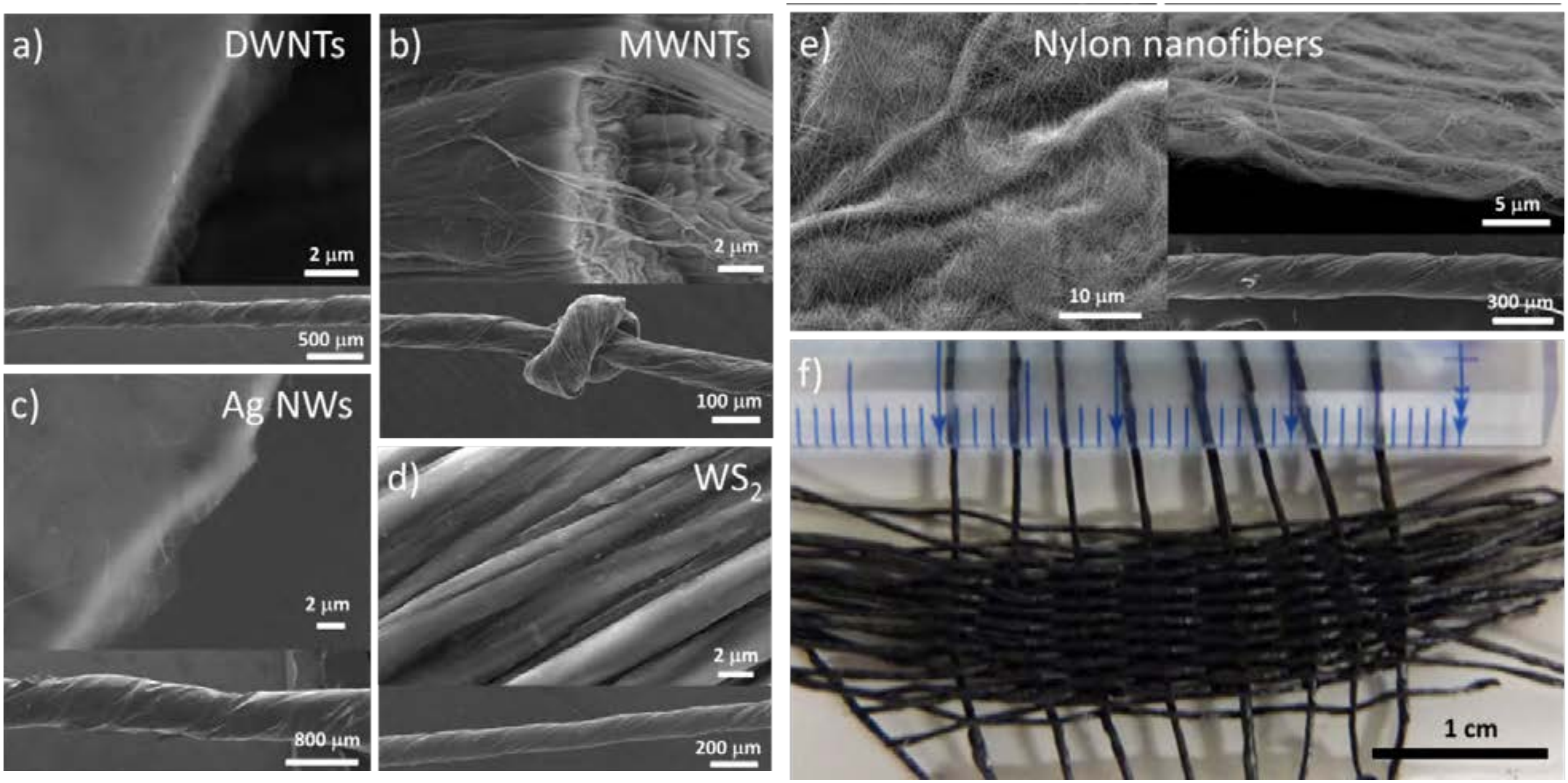
R. Cruz-Silva, et al. ACS Nano 8, 5959-5967 (2014)

GO reduction and grafitization



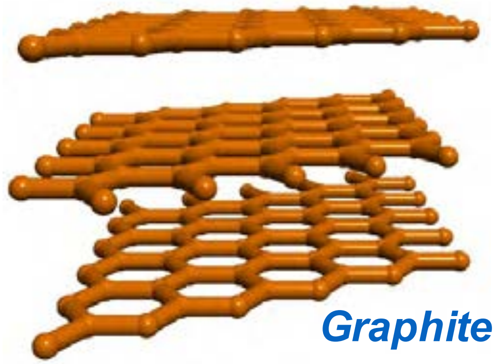
R. Cruz-Silva, et al. ACS Nano 8, 5959-5967 (2014)

Hybrid-Graphene Fibers & Fabrics

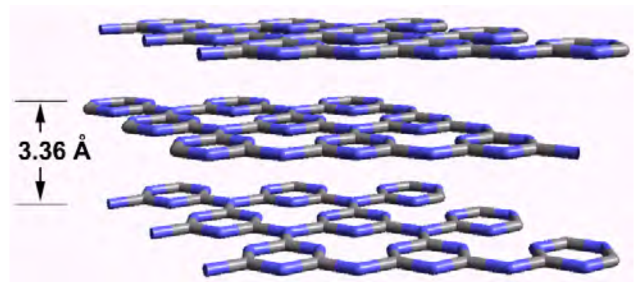


R. Cruz-Silva, et al. ACS Nano 8, 5959-5967 (2014)

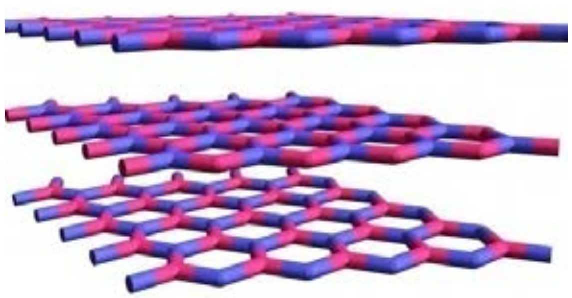
Perfect Layered Materials



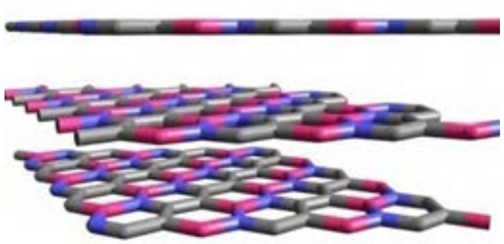
Graphite



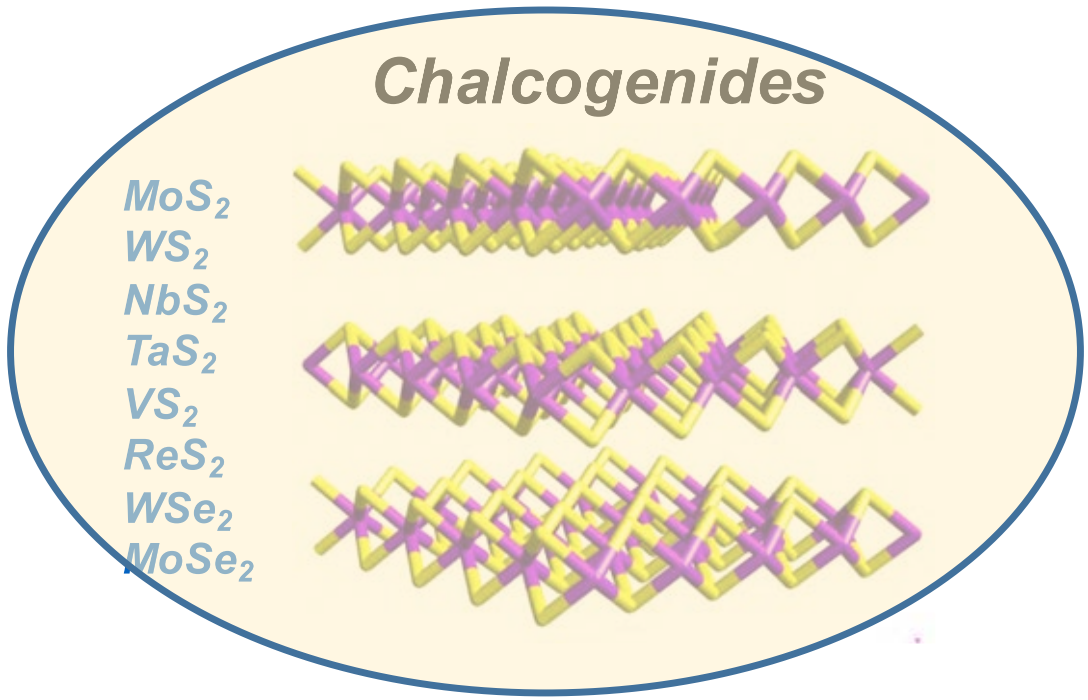
Carbon Nitride



Boron Nitride

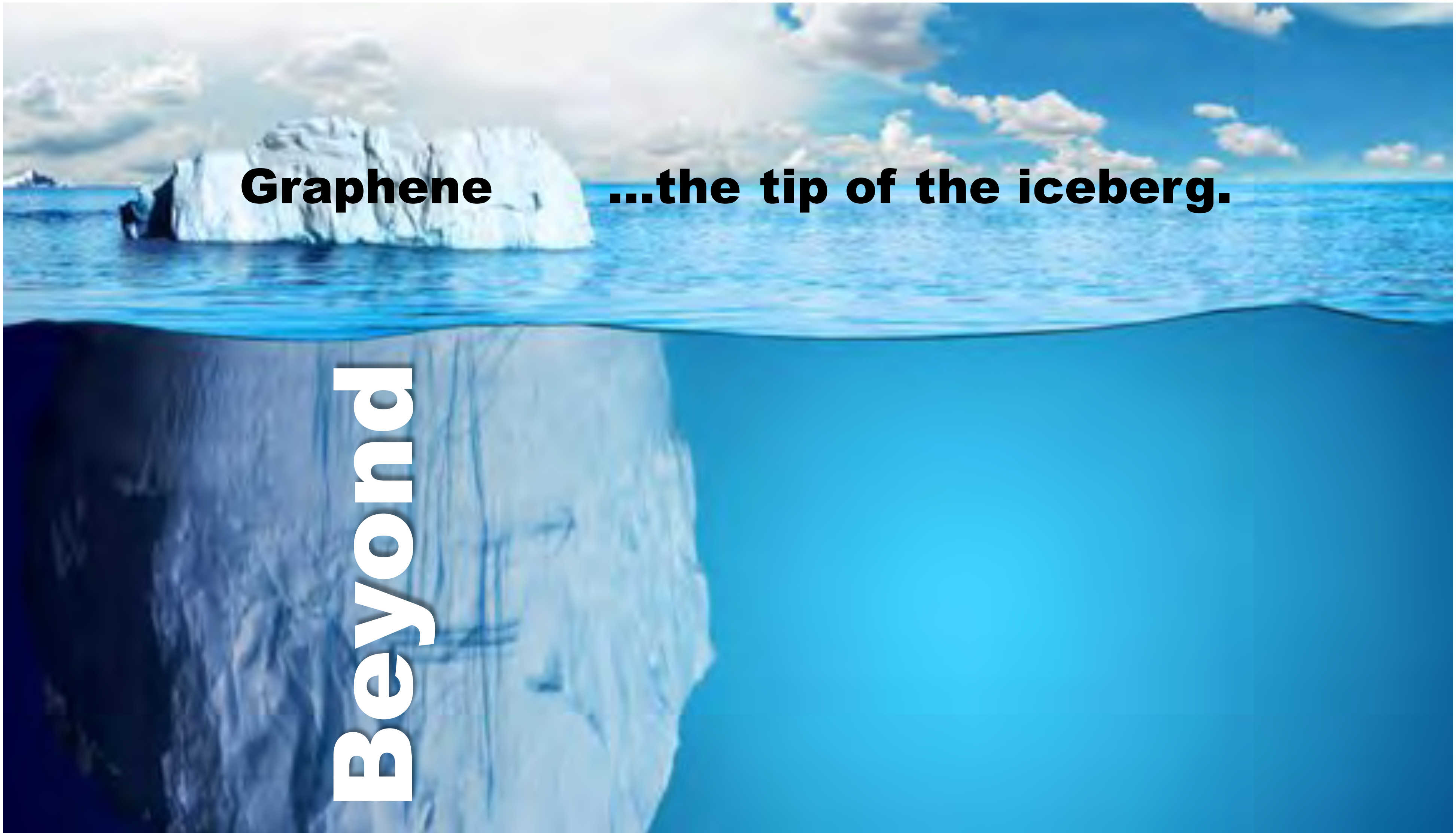


Boron Carbo-Nitride



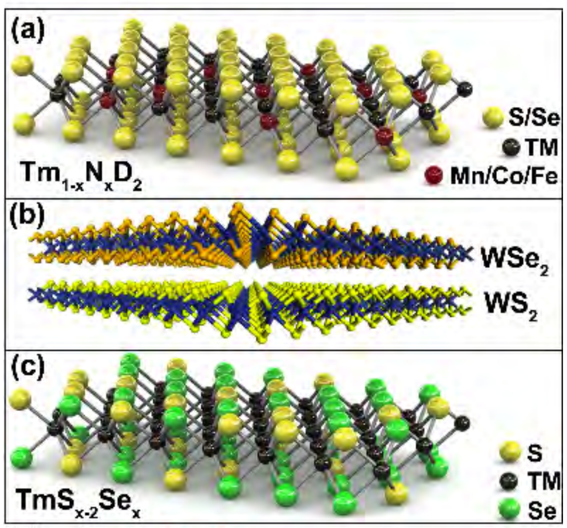
OTHERS VO_5, $NiCl_2$ MgB_2

Beyond Graphene: Layered Materials



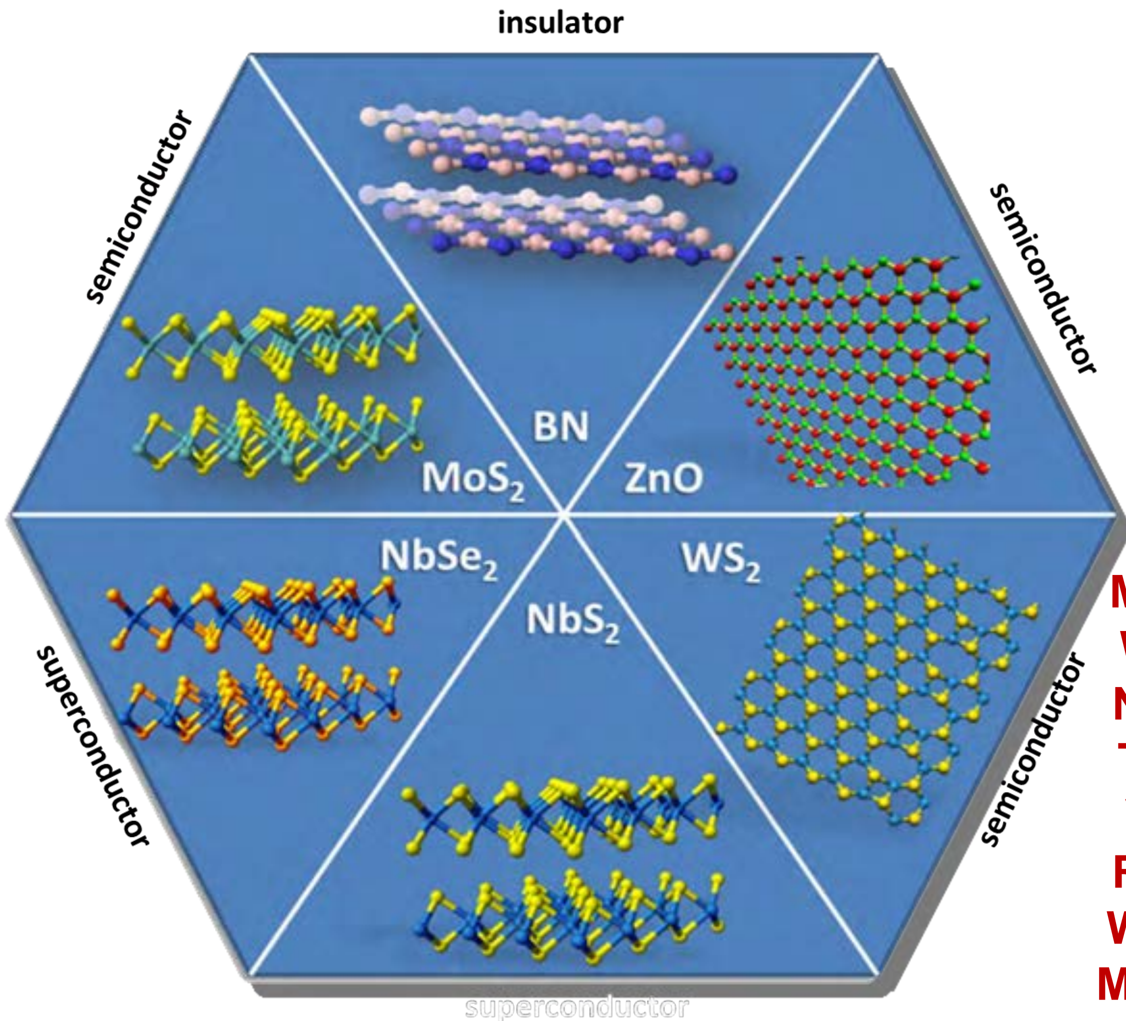
Synthesis and Defect Engineering

Beyond Graphene



Doping Layers
And
Hetero-layers

V_2O_5, $NiCl_2$, MgB_2

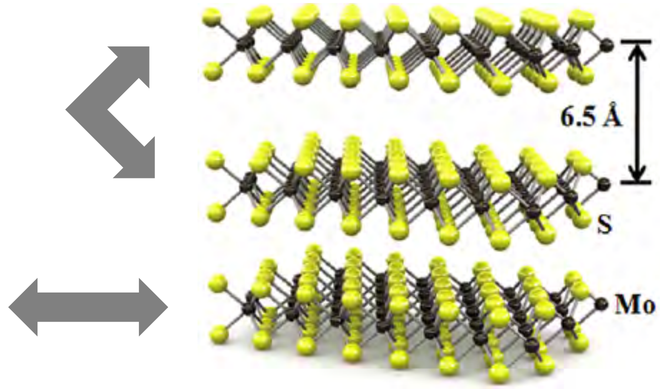


MoS_2
WS_2
NbS_2
TaS_2
VS_2
ReS_2
WSe_2
$MoSe_2$

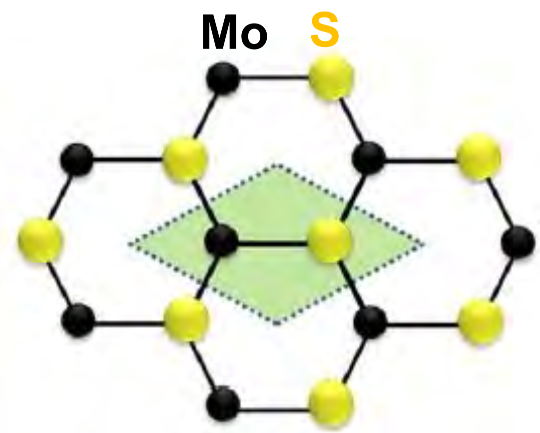
Crystal Structure of MoS_2

vdW bond

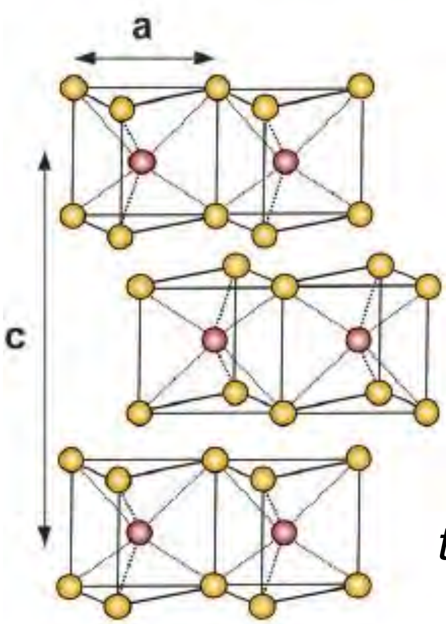
covalent bond

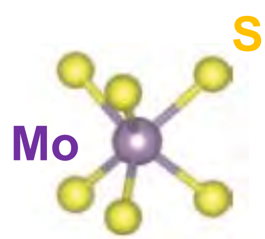


Layered structure



top view





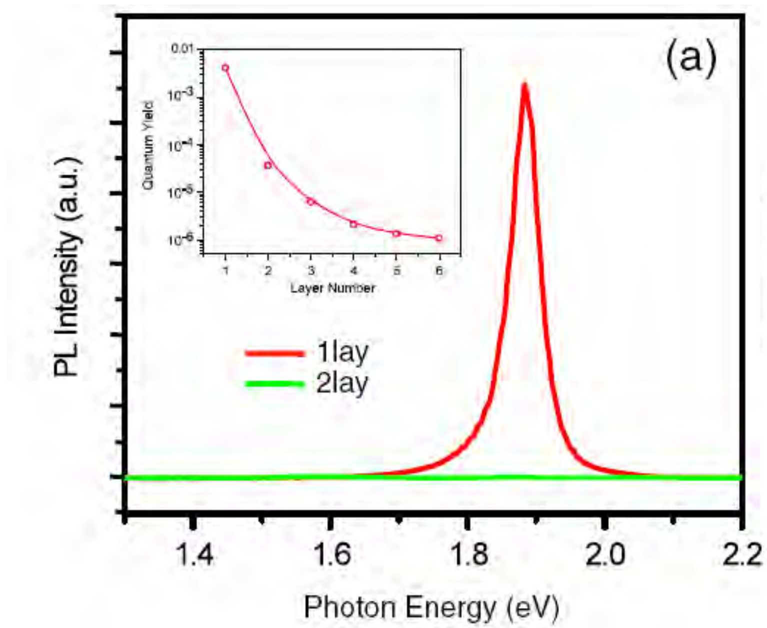
1H single layer MoS_2 with trigonal prismatic coordination (D_{3h})

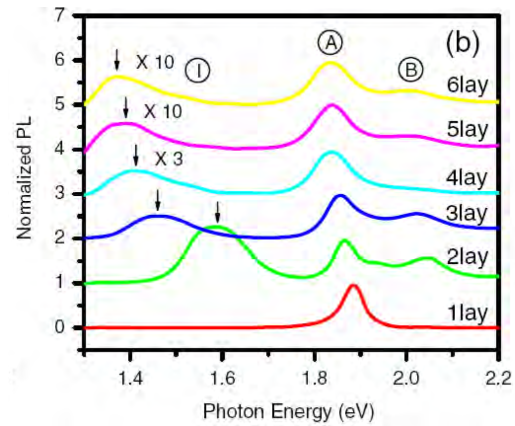
No. of layer	Point group
odd	D_{3h}
even	D_{3d}
bulk	D_{6h}

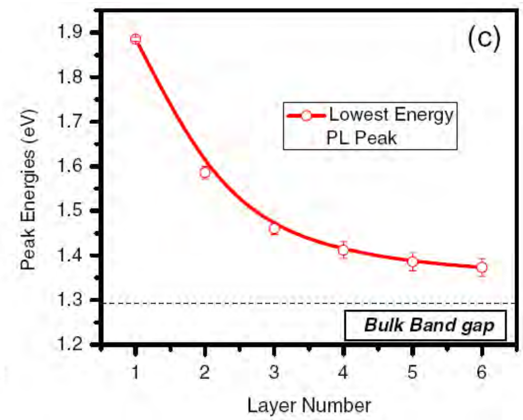
Bulk MoS_2 in 2H phase
2: 2 layers per repeat unit
H: Hexagonal symmetry

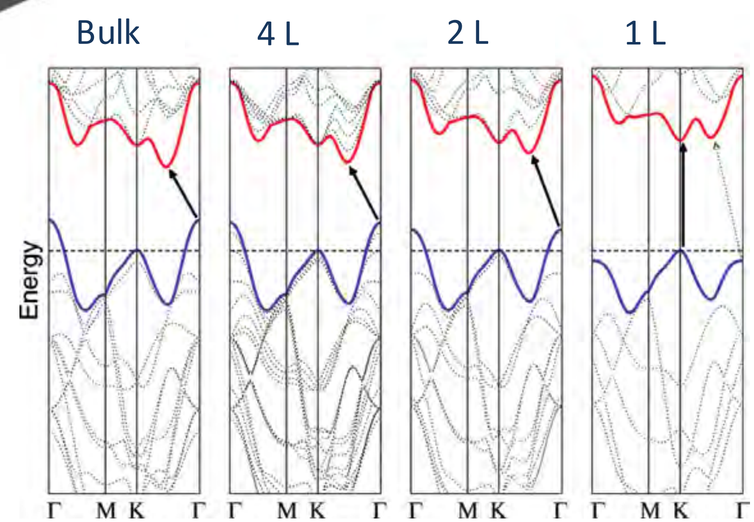
Chhowalla, et al. Nat. Chem. 5 (2013) 263.
Xu, et al. Chem. Rev. 113 (2013) 3766.
Huang, et al. Chem. Soc. Rev. 42 (2013) 1934.
Terrones, et al. Sci. Rep. 4 (2014) 4215.

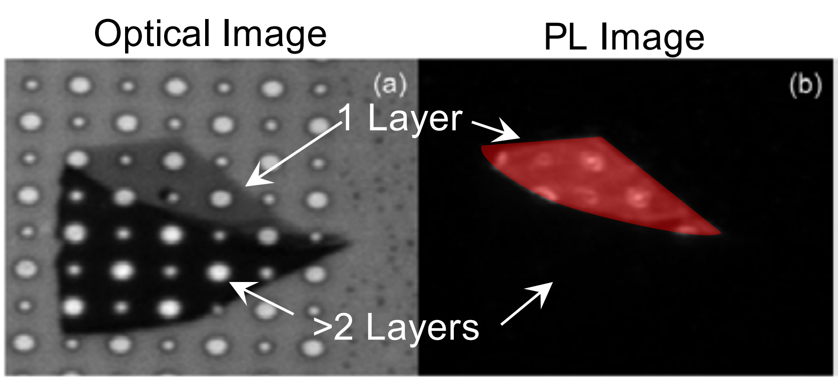
Exfoliated MoS_2: Photoluminescence







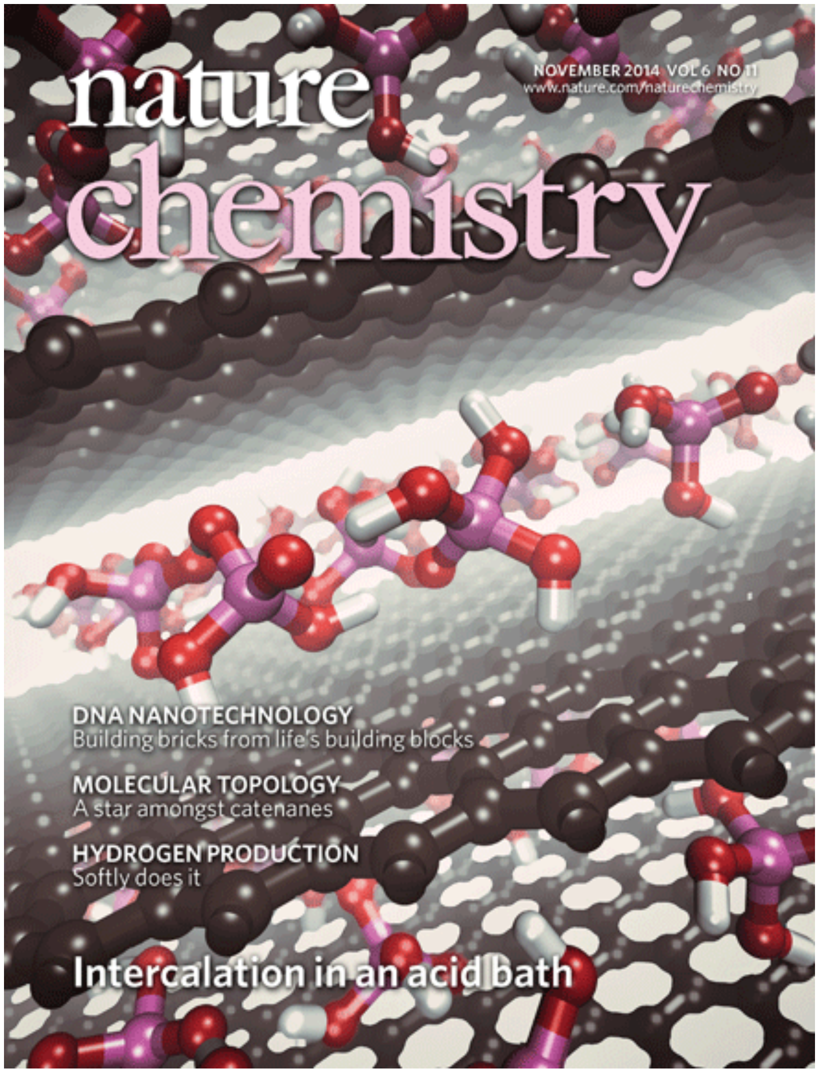


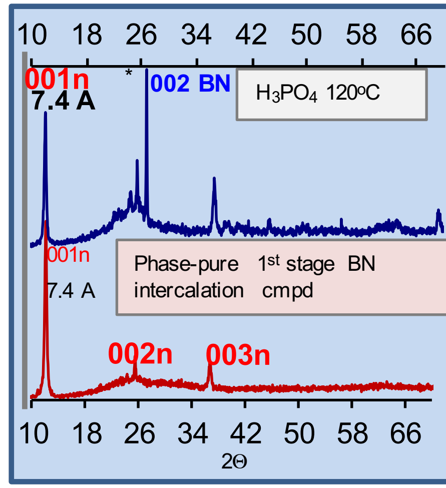


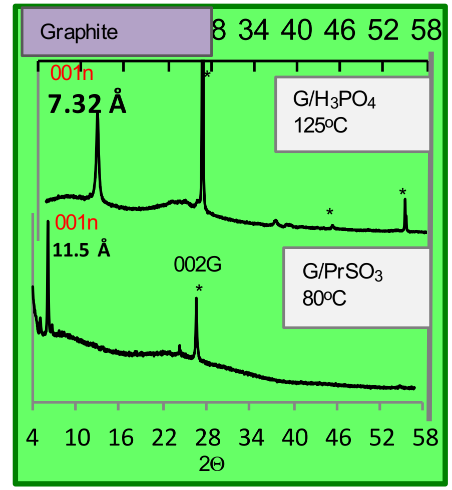
Splendiani A. *et al. Nano Letters* **10**, p1271 (2010)

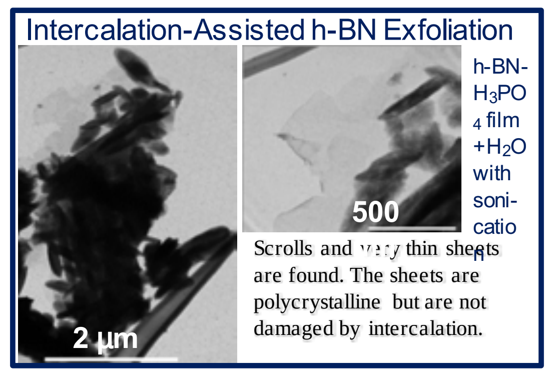
Mak K. F. *et al. Phys. Rev. Lett.* **105**, 136805 (2010)

Intercalation and Exfoliation of h-BN and Graphite



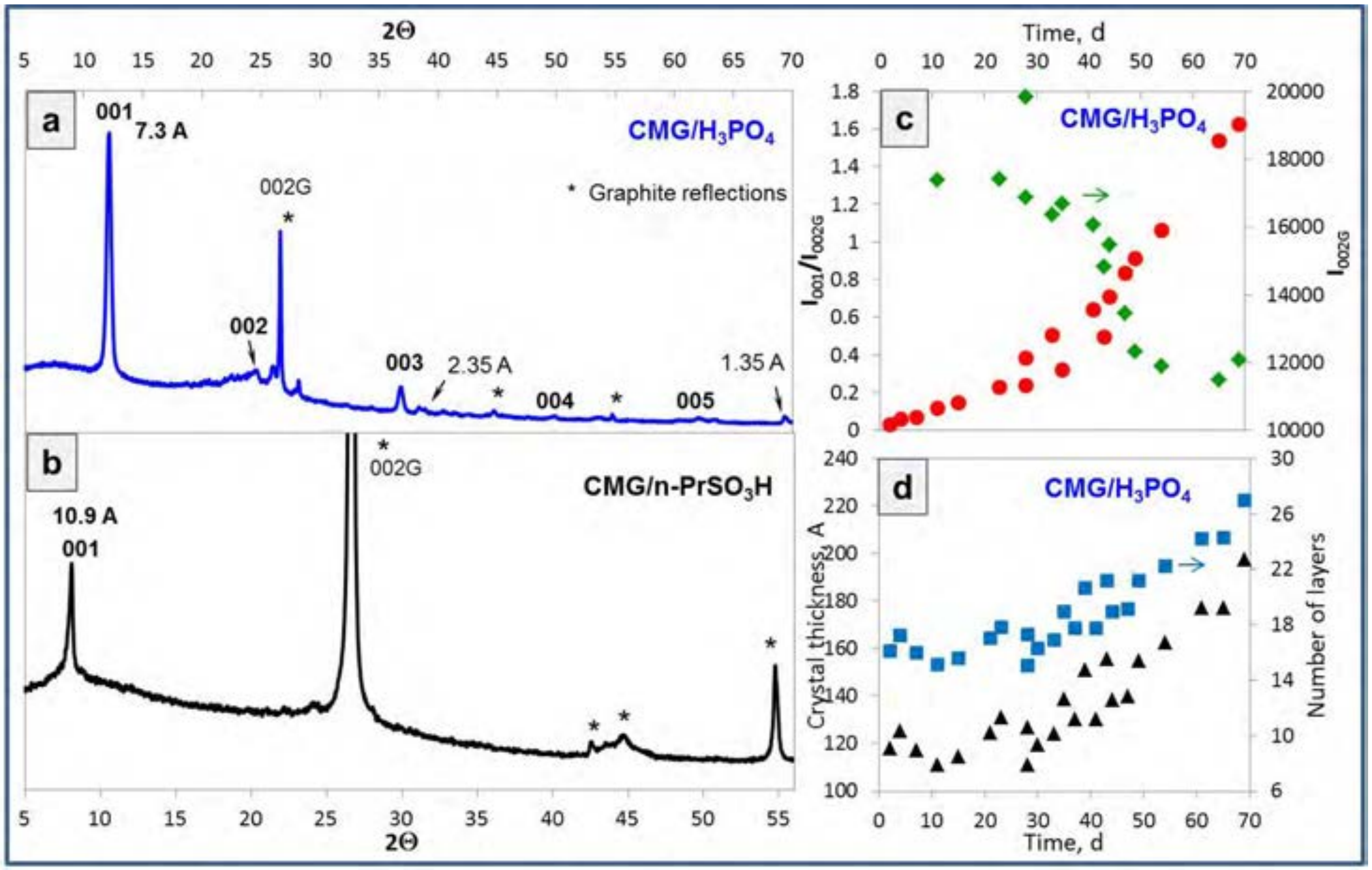






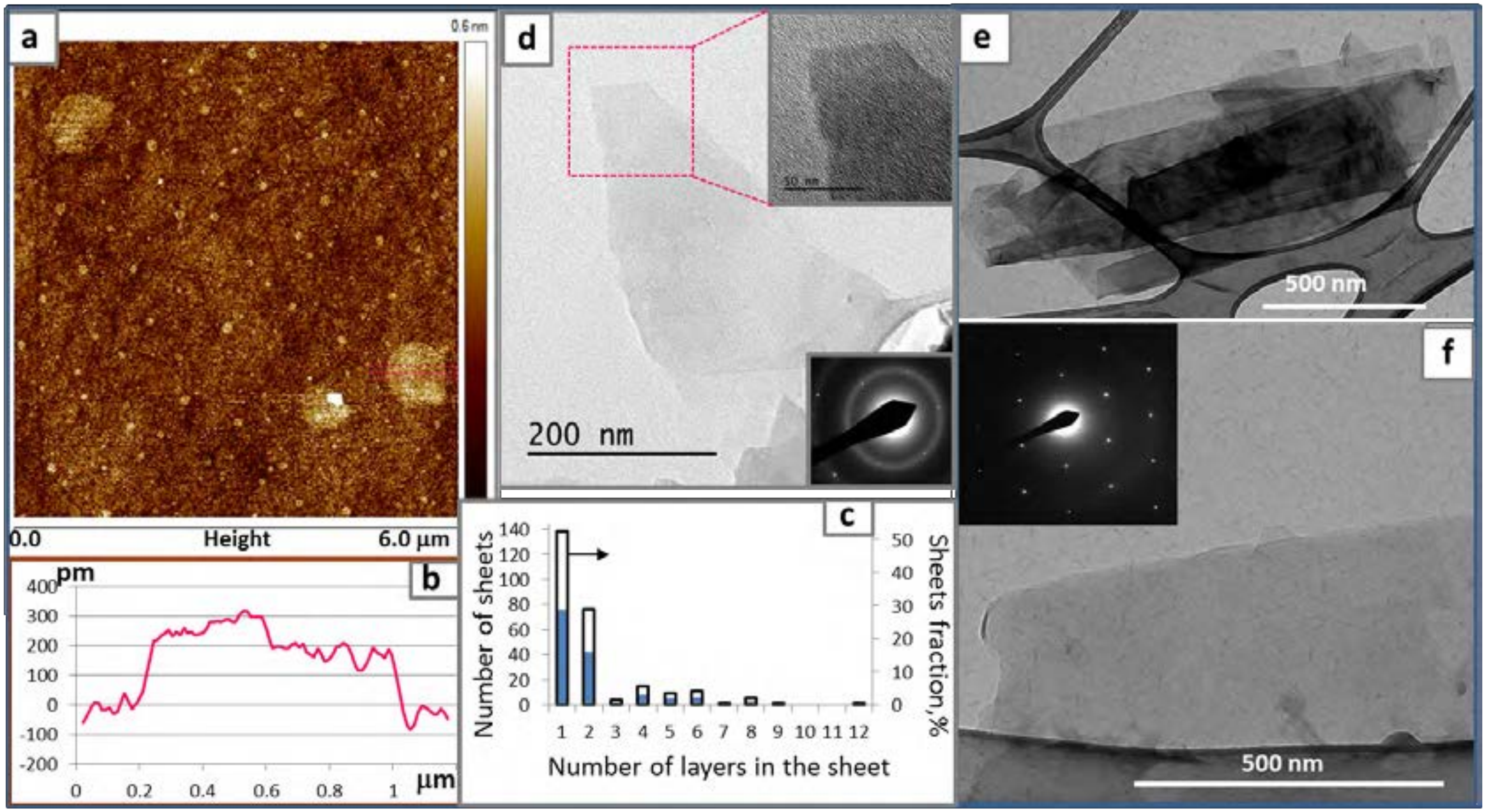
Mallouk, Crespi, Terrones
N. Kovtyukhova *JACS* 135, 8372 (2013)
N. Kovtyukhova *Nature Chemistry* (2014)

New Result: Intercalation and Exfoliation of Grahphite using Brønsted Acids



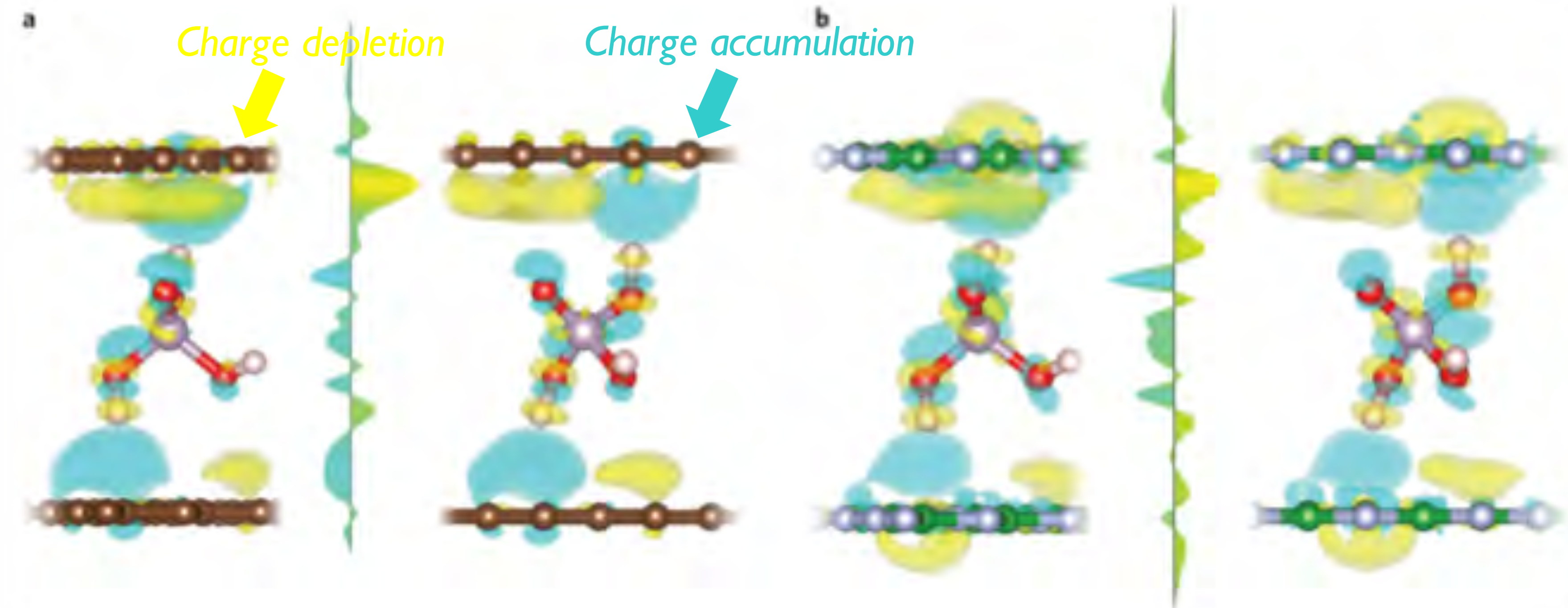
Mallouk, Crespi, Terrones
N. Kovtyukhova *Nature Chemistry* (2014)

New Result: Intercalation and Exfoliation of Grahphite using Brønsted Acids



Mallouk, Crespi, Terrones
N. Kovtyukhova *Nature Chemistry* (2014)

Differential Charge Density Map: Intercalation of Graphite and BN with H_3PO_4

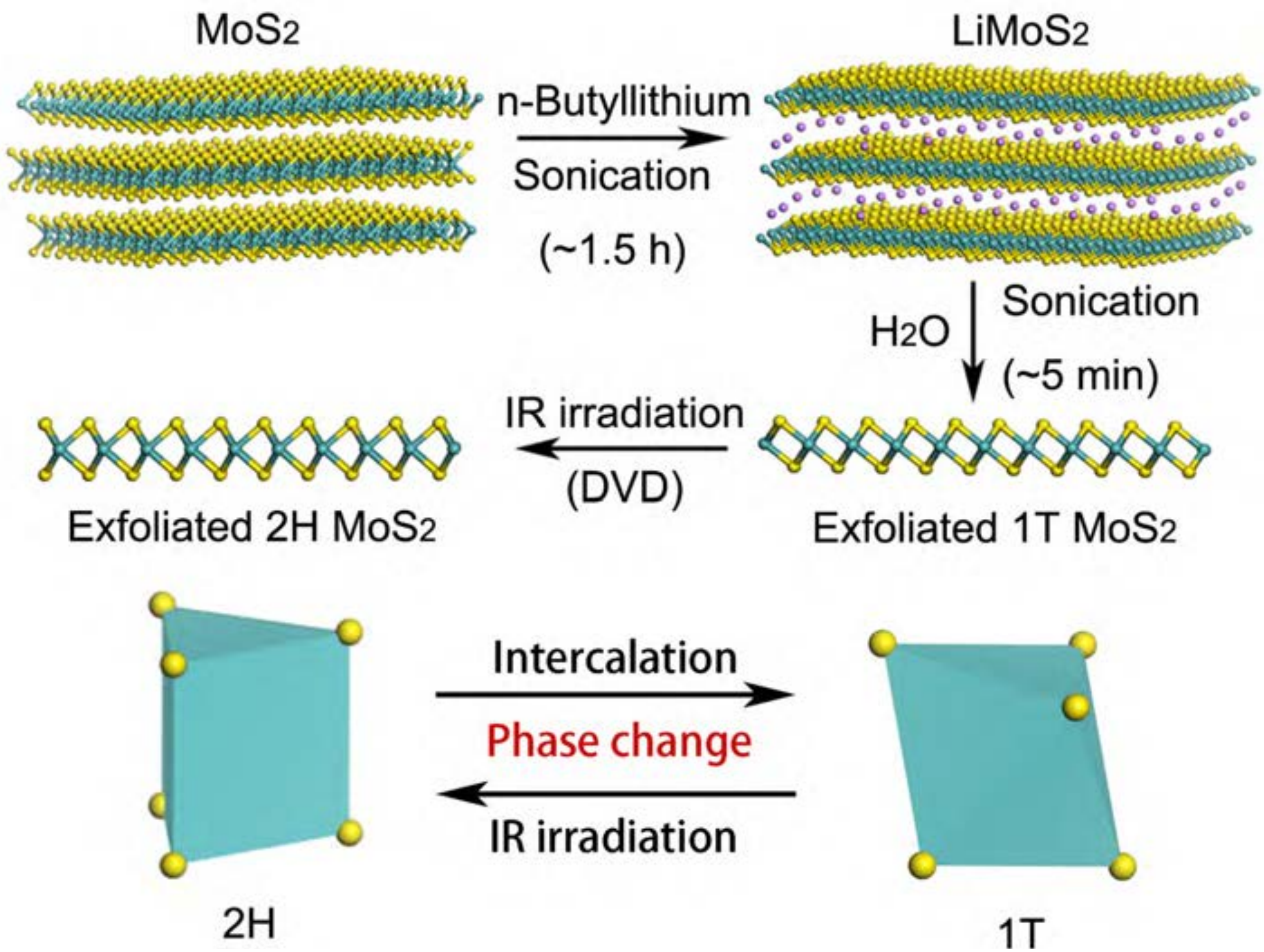


Graphite **Hexagonal Boron Nitride**

Strong dipolar interactions between the guest molecules and the graphite or boron nitride sheets. Cyan and yellow indicate charge accumulation and depletion, respectively. Color coding of atoms: carbon (brown), oxygen (red), hydrogen (white), phosphorus (pink), boron (green), nitrogen (light grey).

N. Kovtyukhova *Nature Chemistry* (2014)

Intercalation and Exfoliation of MoS_2 with Li, sonication and IR irradiation



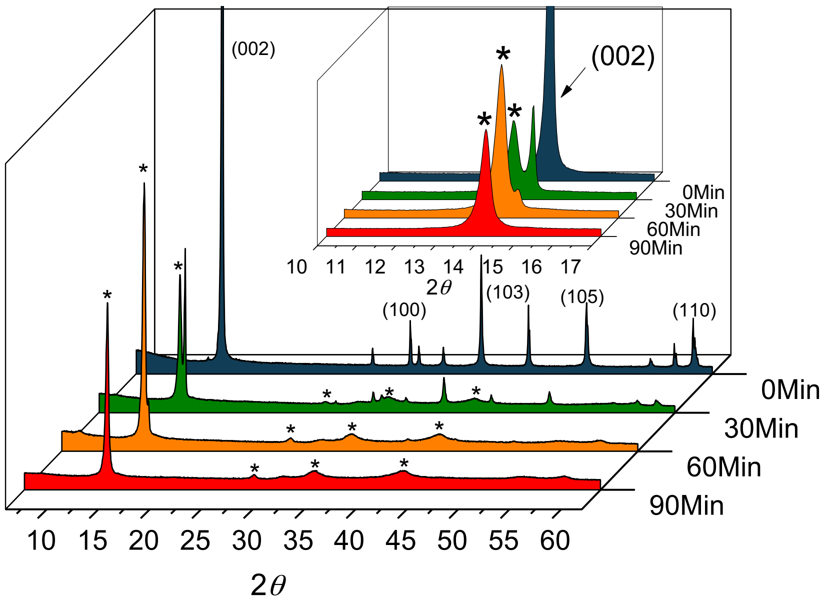
X. Fan, P. Xu, D. Zhou, Y. Sun, Y. C. Li, M.A.T. Nguyen, M. Terrones, T.E. Mallouk.
Nano Letters doi:10.1021/acs.nanolett.5b02091 (2015)

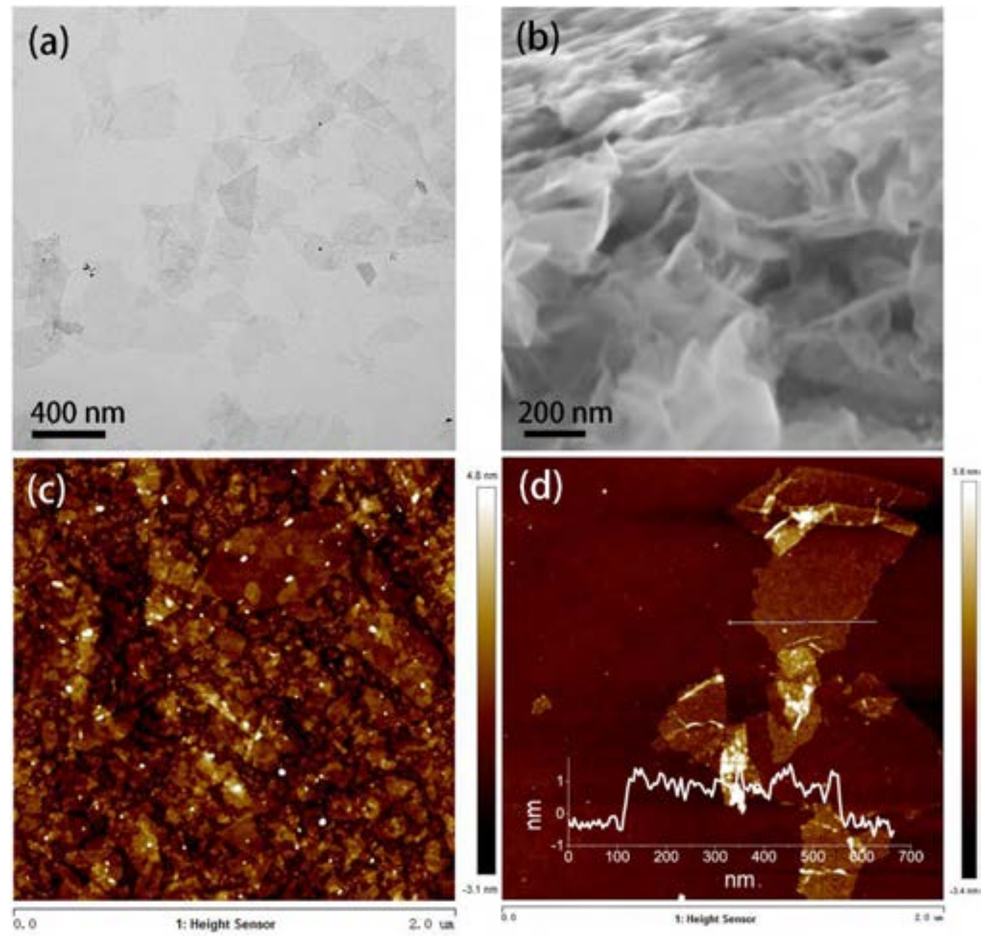
PENNSTATE

MRI MATERIALS RESEARCH INSTITUTE

Center for 2-Dimensional and Layered Materials Penn State

Intercalation and Exfoliation of MoS_2 with Li, sonication and IR irradiation





X. Fan, P. Xu, D. Zhou, Y. Sun, Y. C. Li, M.A.T. Nguyen, M. Terrones, T.E. Mallouk.
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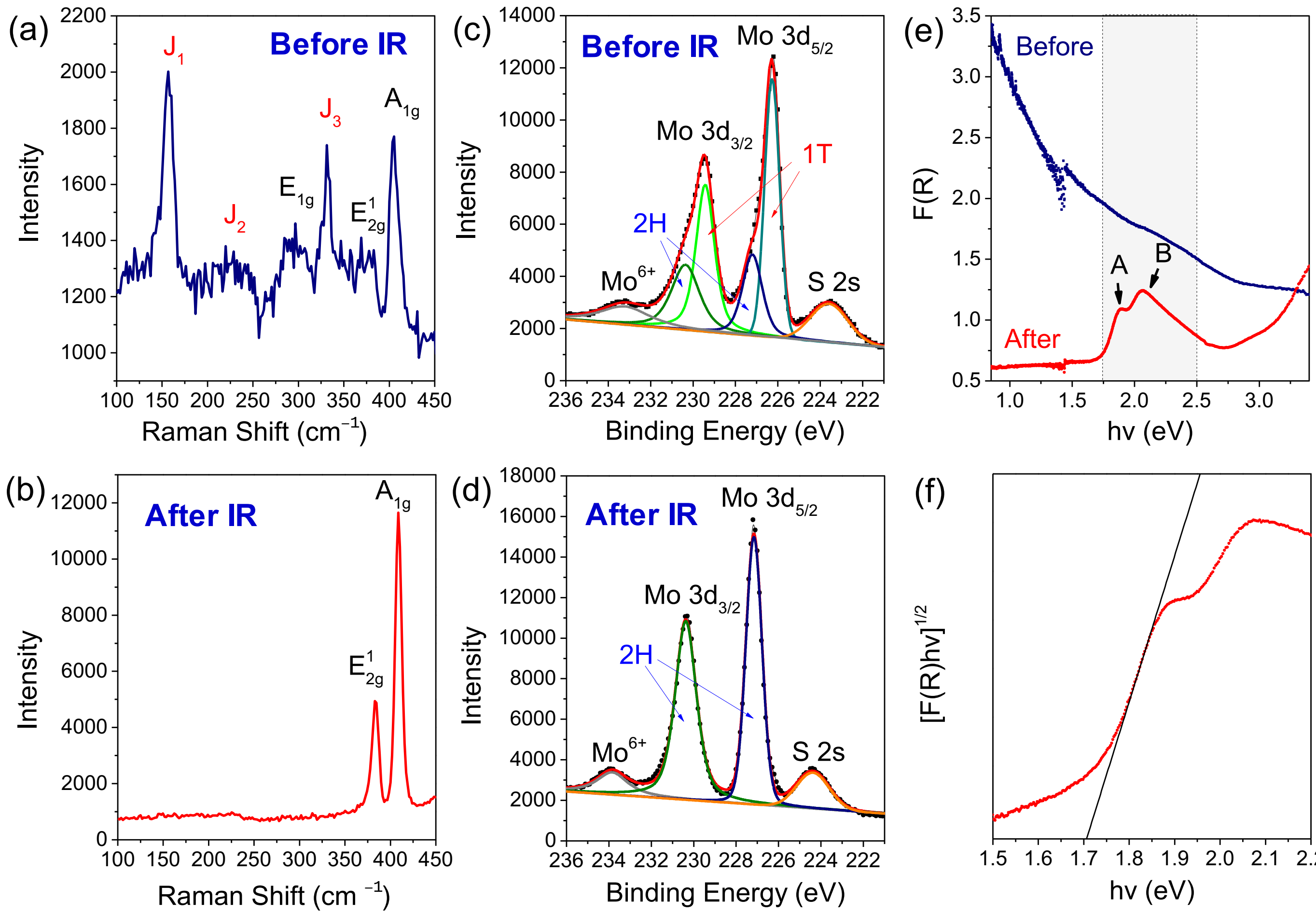
Intercalation and Exfoliation of MoS_2 with Li, sonication and IR irradiation



X. Fan, P. Xu, D. Zhou, Y. Sun, Y. C. Li, M.A.T. Nguyen, M. Terrones, T.E. Mallouk.
Nano Letters doi:10.1021/acs.nanolett.5b02091 (2015)

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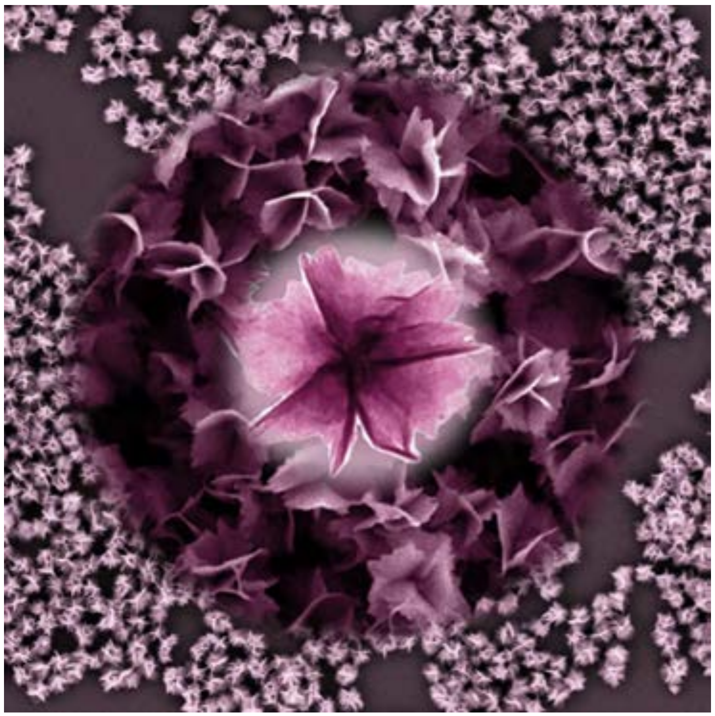
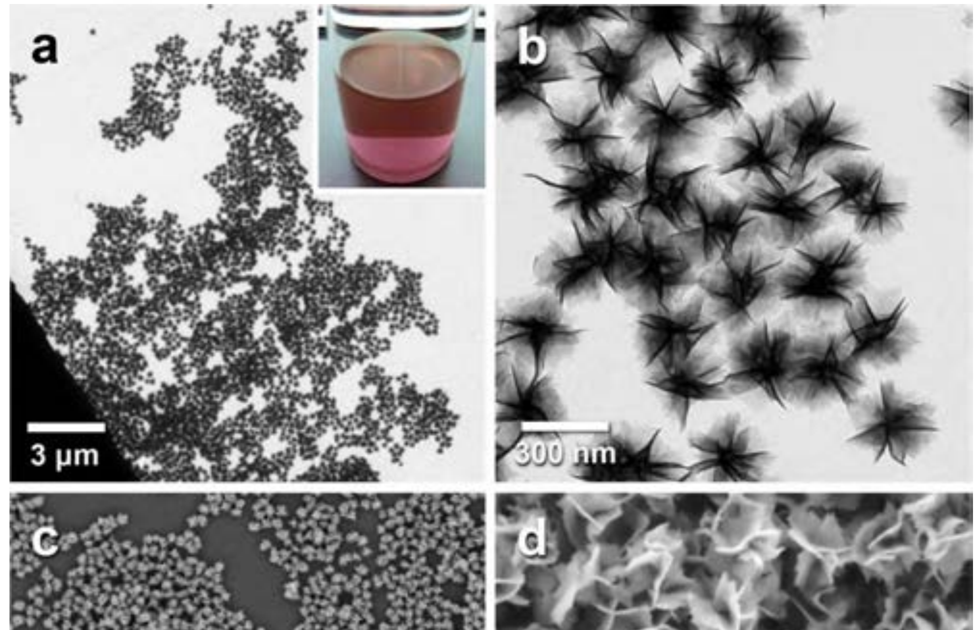
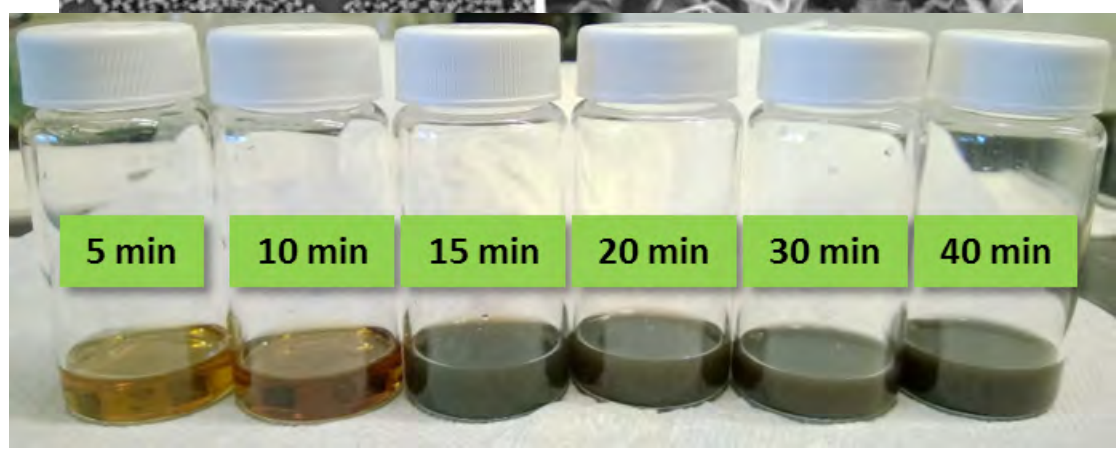
Penn State

Bottom Up: Chemical Synthesis of $MoSe_2$ Nanoflowers

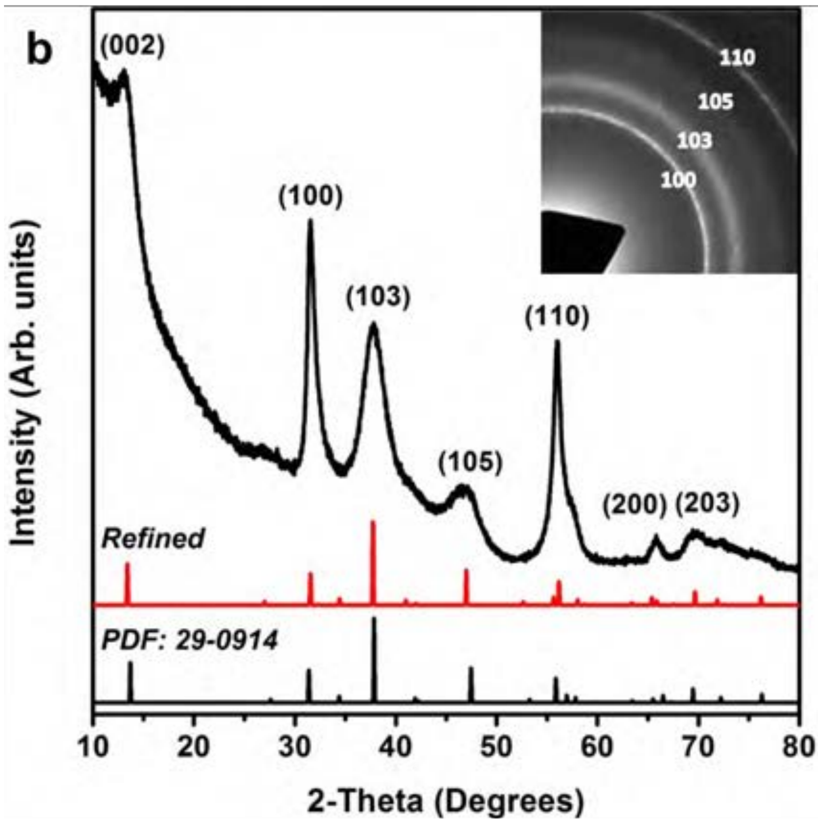


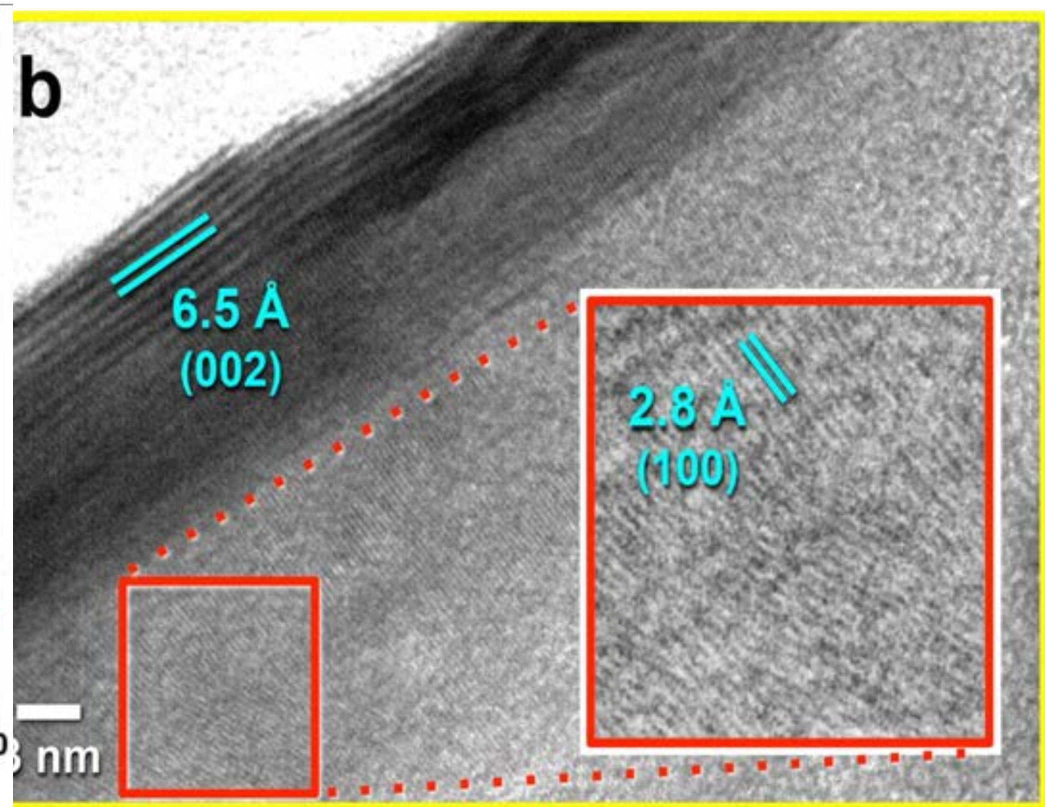




Schaak & Terrones
Chem. Mater. (2015)

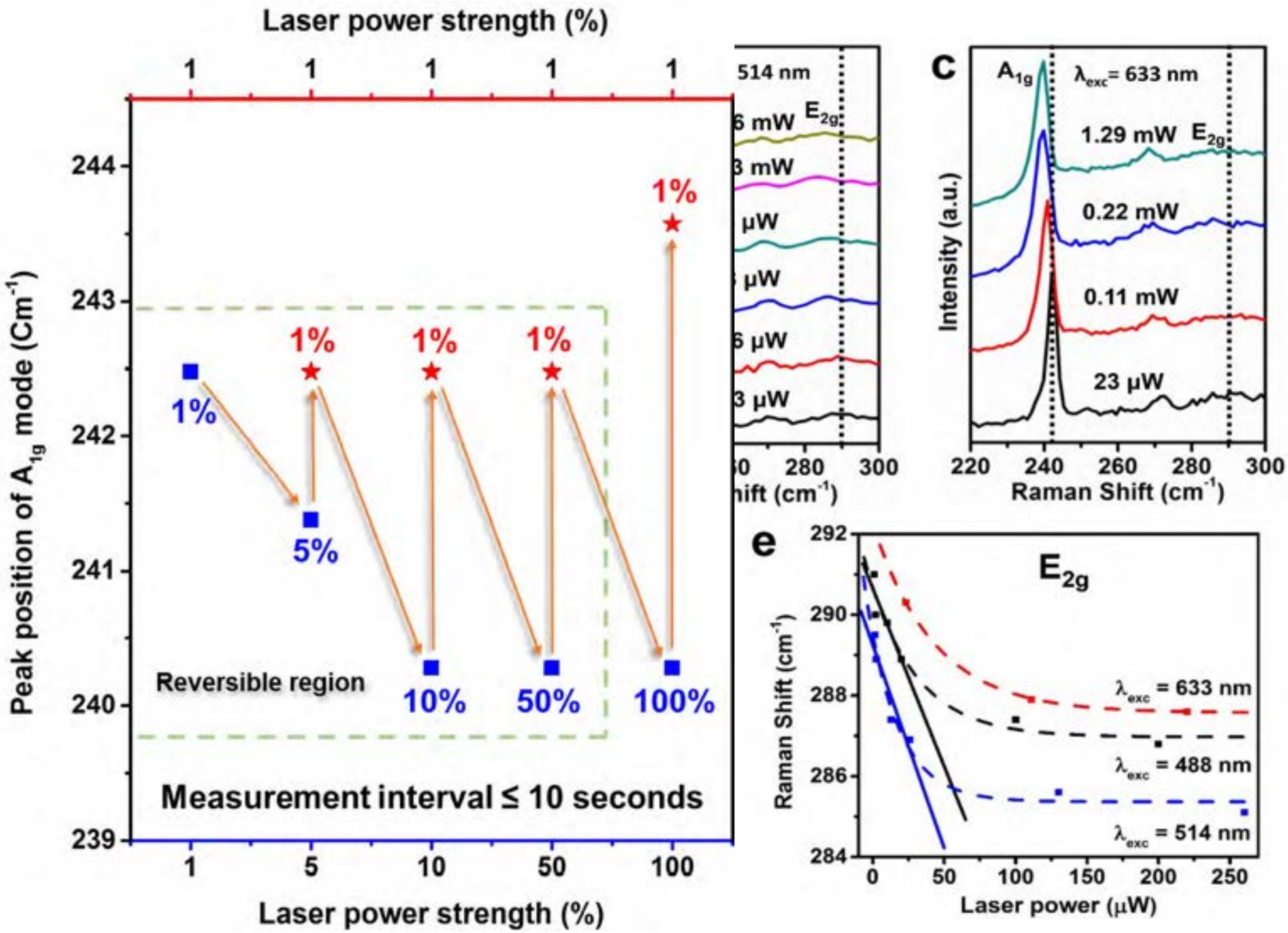
Bottom Up: Chemical Synthesis of $MoSe_2$ Nanoflowers





Schaak & Terrones
Chem. Mater. (2015)

Bottom Up: Chemical Synthesis of $MoSe_2$ Nanoflowers



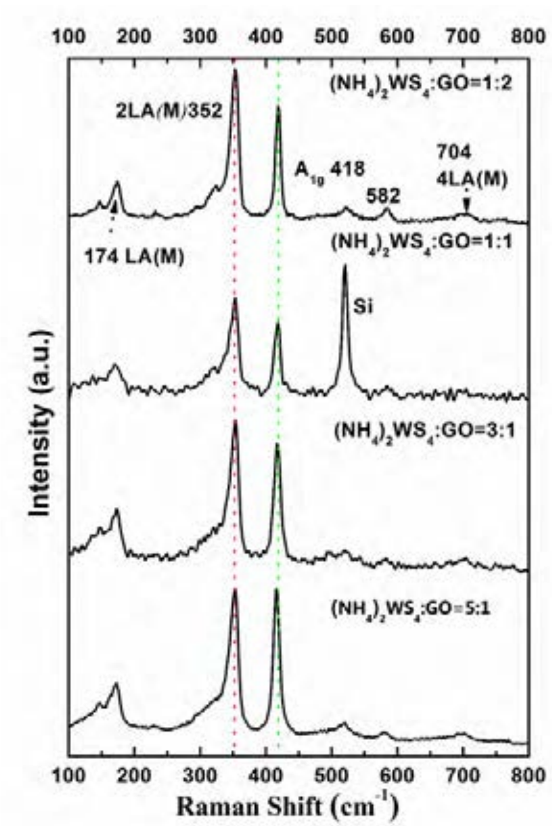
Schaak & Terrones. Chem. Mater. (2015)

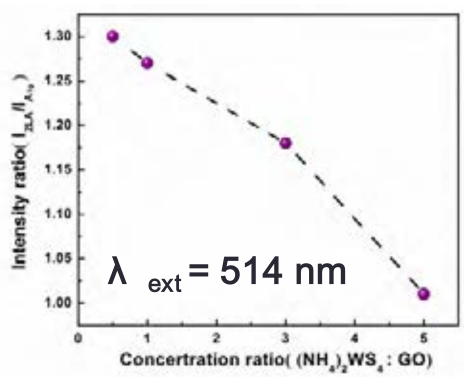
Heterostructures of TMDs and Graphene by Wet Chemistry

Center for 2-Dimensional and Layered Materials Penn State

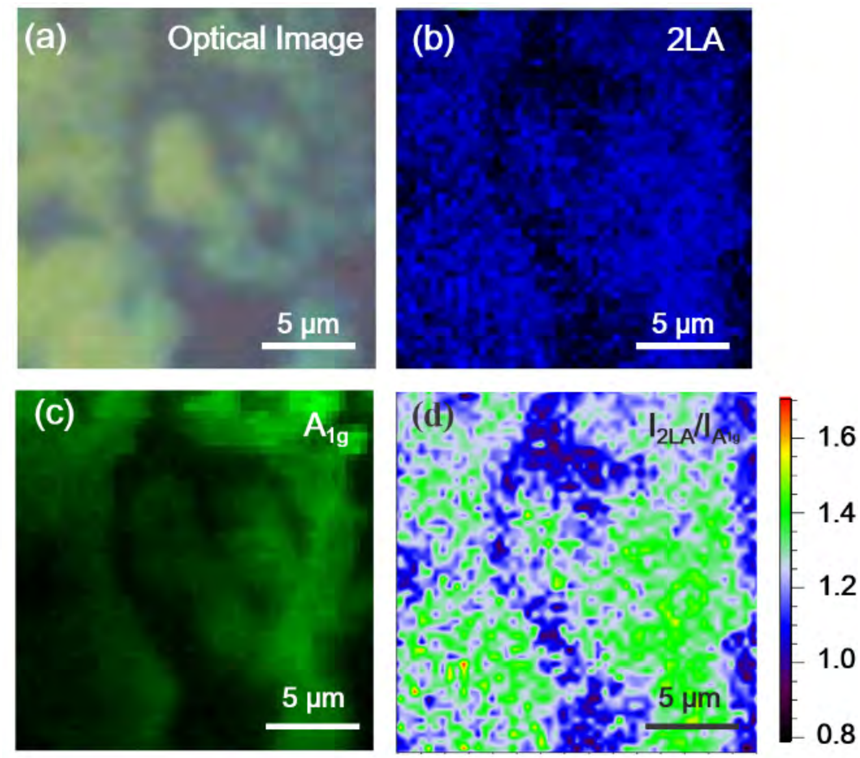
PENNSTATE 1855

➢ Raman Spectroscopy of WS_2/Graphene





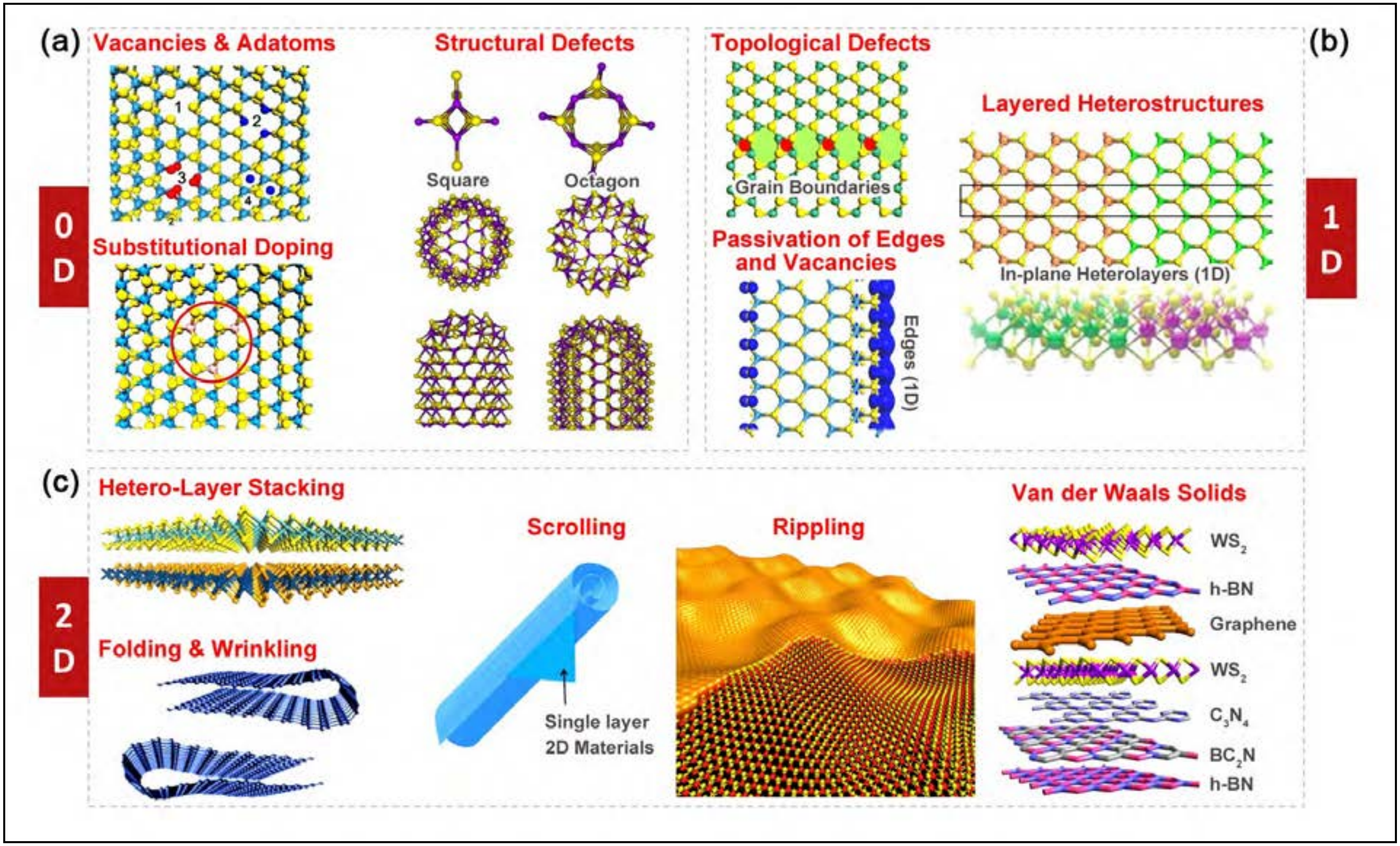
➢ Raman mapping of WS_2/Graphene



The obtained I_{2LA}/I_{A1g} ratios range from 1.00 to 1.33, suggesting the existence of mono- and bi-layered WS_2

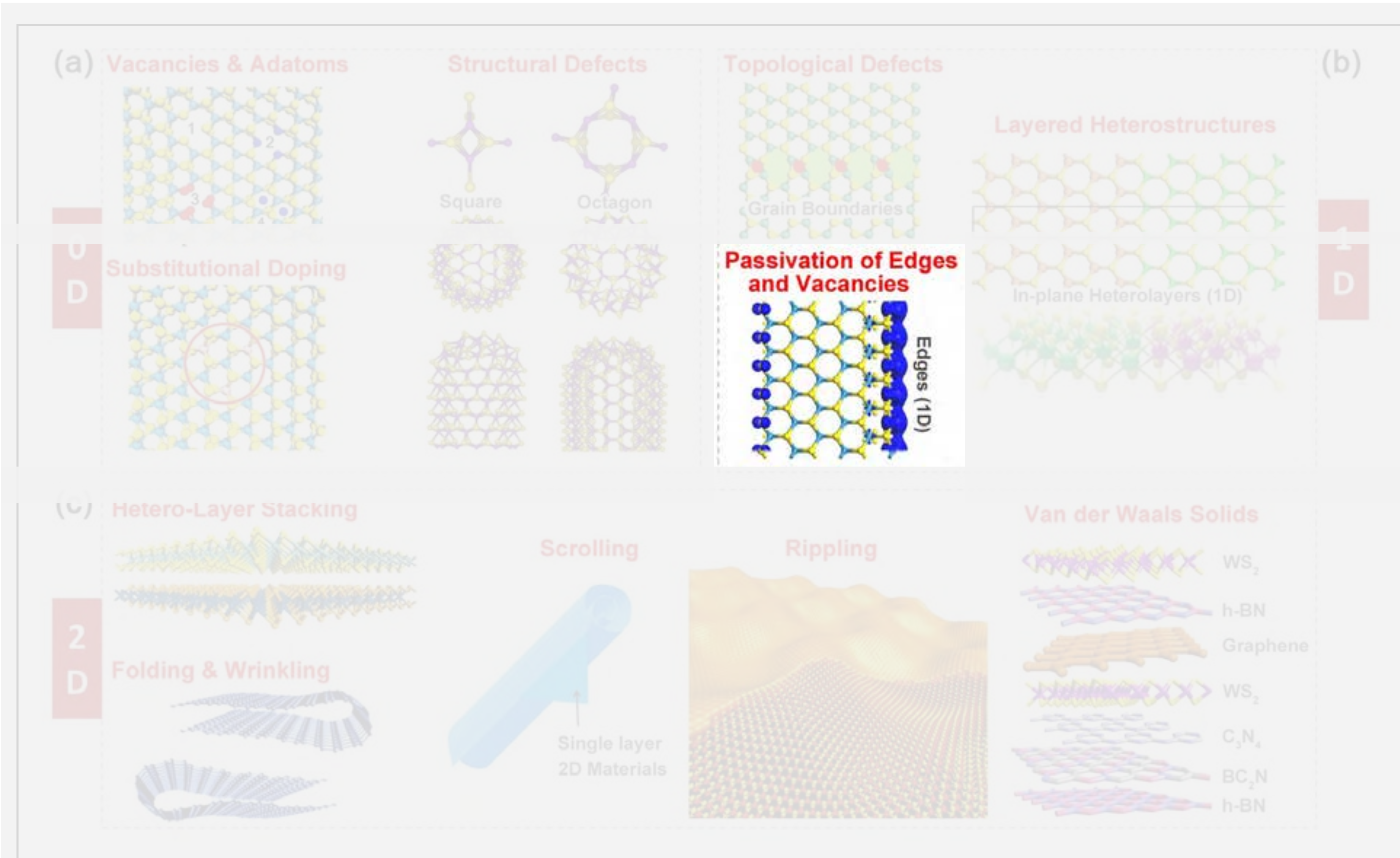
Yu Lei, M. Terrones, et al., unpublished (2015)

Defect Engineering



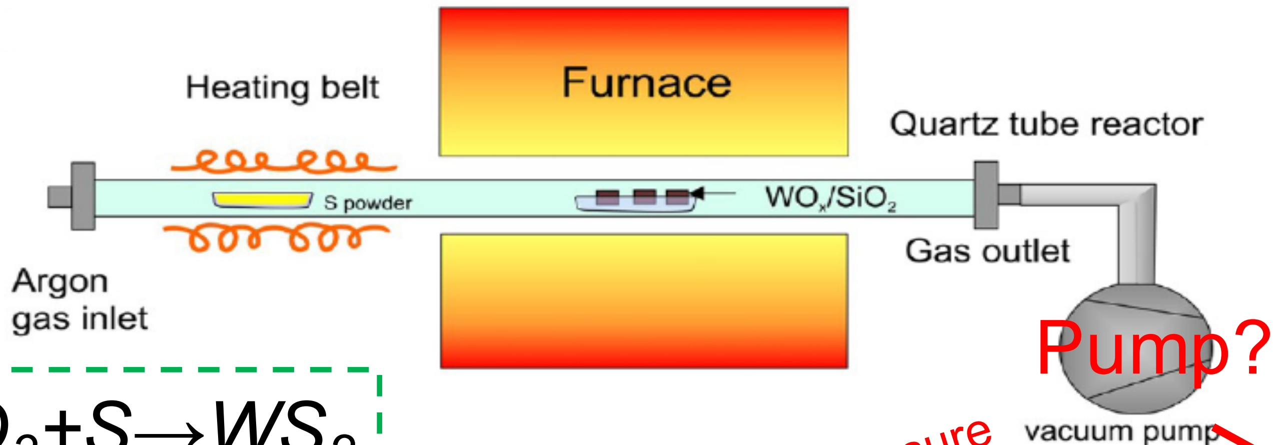
Z. Lin, B.R. Carvalho, E. Kahn, R. Lv, R. Rao, H. Terrones, M.A. Pimenta, M. Terrones. 2D Materials (2016)

Defect Engineering



Z. Lin, B.R. Carvalho, E. Kahn, R. Lv, R. Rao, H. Terrones, M.A. Pimenta, M. Terrones. 2D Materials (2016)

Synthesis of WS_2 monolayers with CVD
---- from islands and edges to films



Pump?

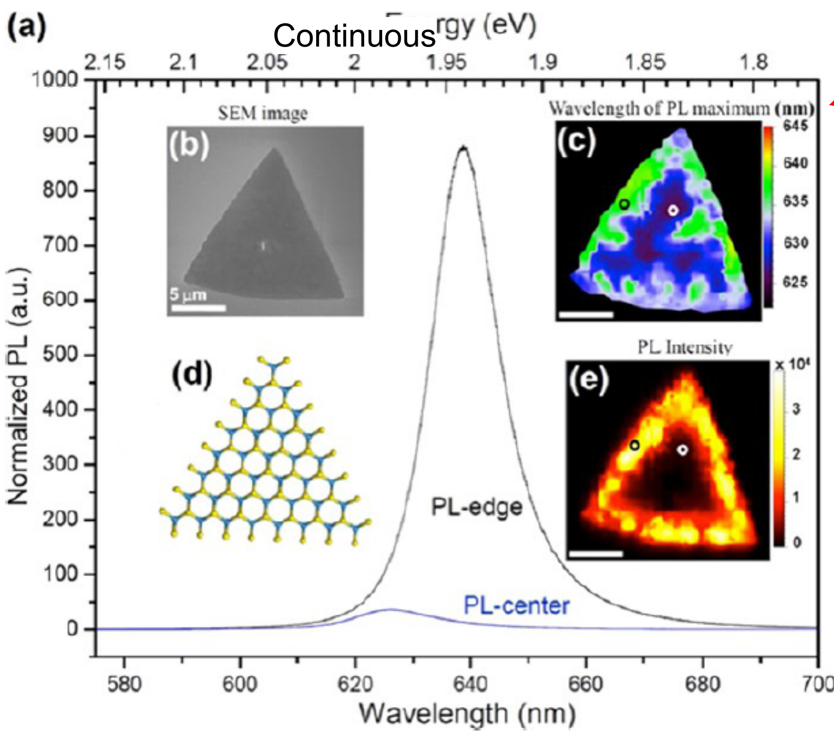
$$WO_3 + S \rightarrow WS_2$$

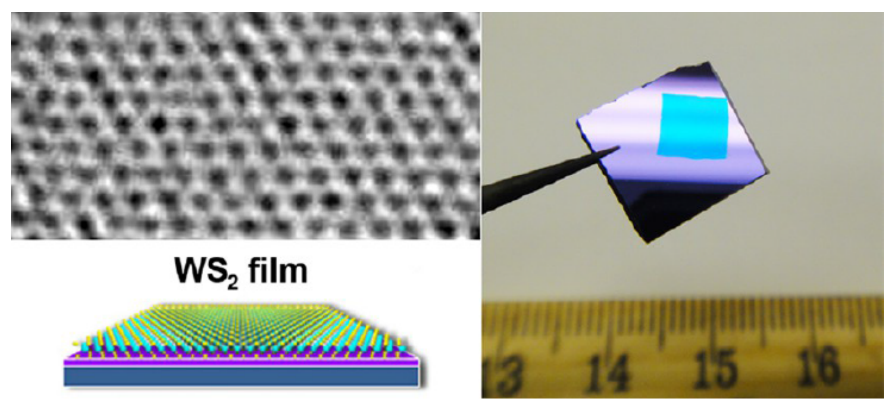
Ambient pressure

Triangular islands

Low pressure

Continuous films

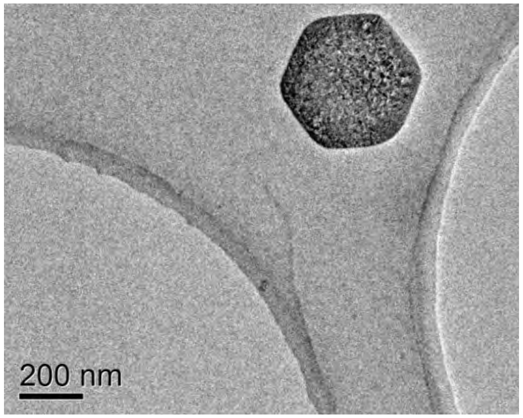


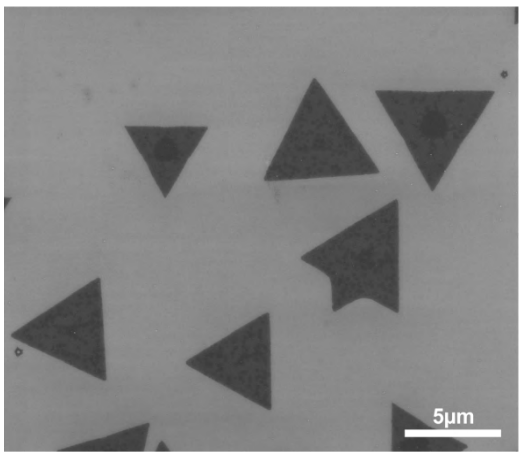


Gutiérrez, et al. Nano Lett. 13 (2013) 3447.
Elías, et al. ACS Nano 7 (2013) 5235.
Butler, et al. ACS Nano 7 (2013) 2898.

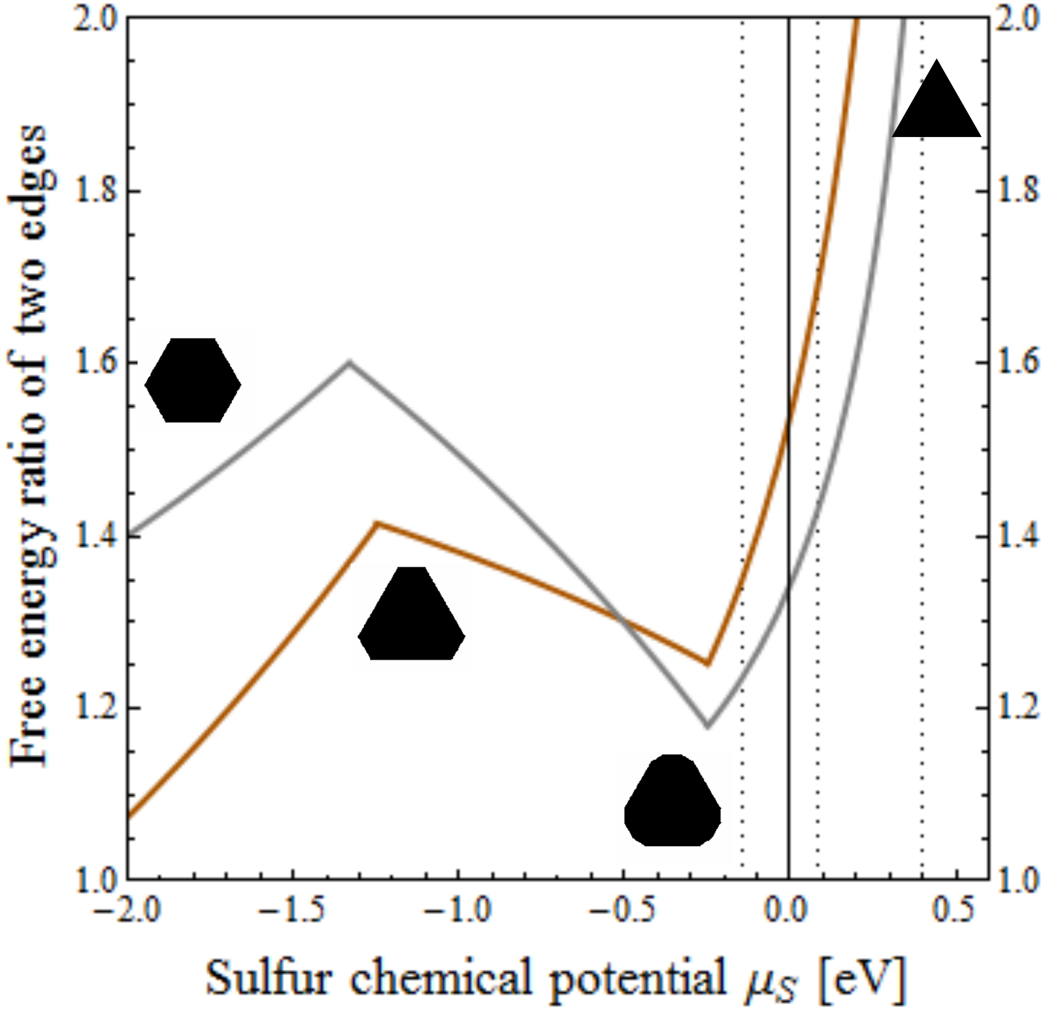
Hexagonal Islands of WS_2

Terrones & Crespi





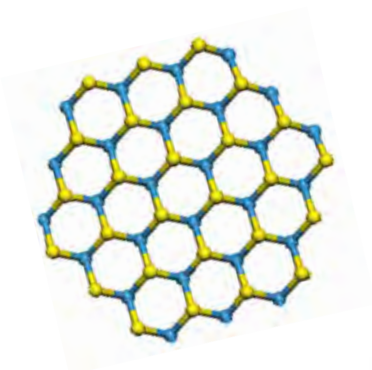
Y. Wang, A. Berkdemir, unpublished (2013)

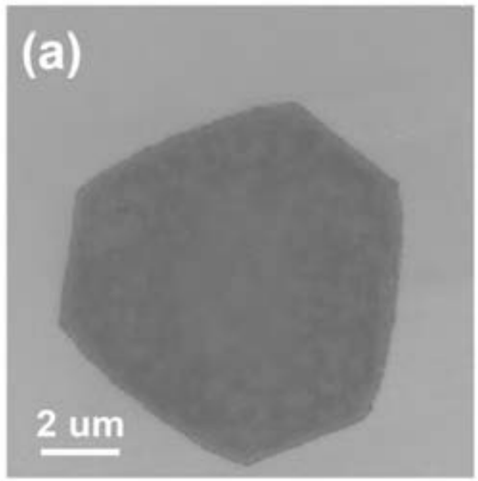


A. Berkdemir, et al. (Unpublished)

SEM and PL of Hexagonal Islands of WS_2

Terrones & Crespi

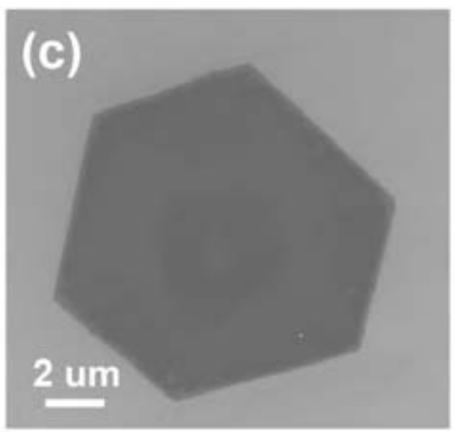


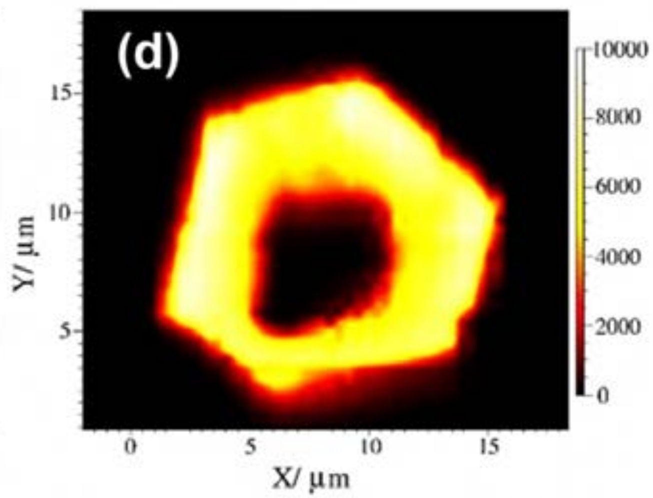


- **Questions remaining for theory and experiment**

What is the edge structure of these hexagonal islands?

Is the edge termination the key parameter?

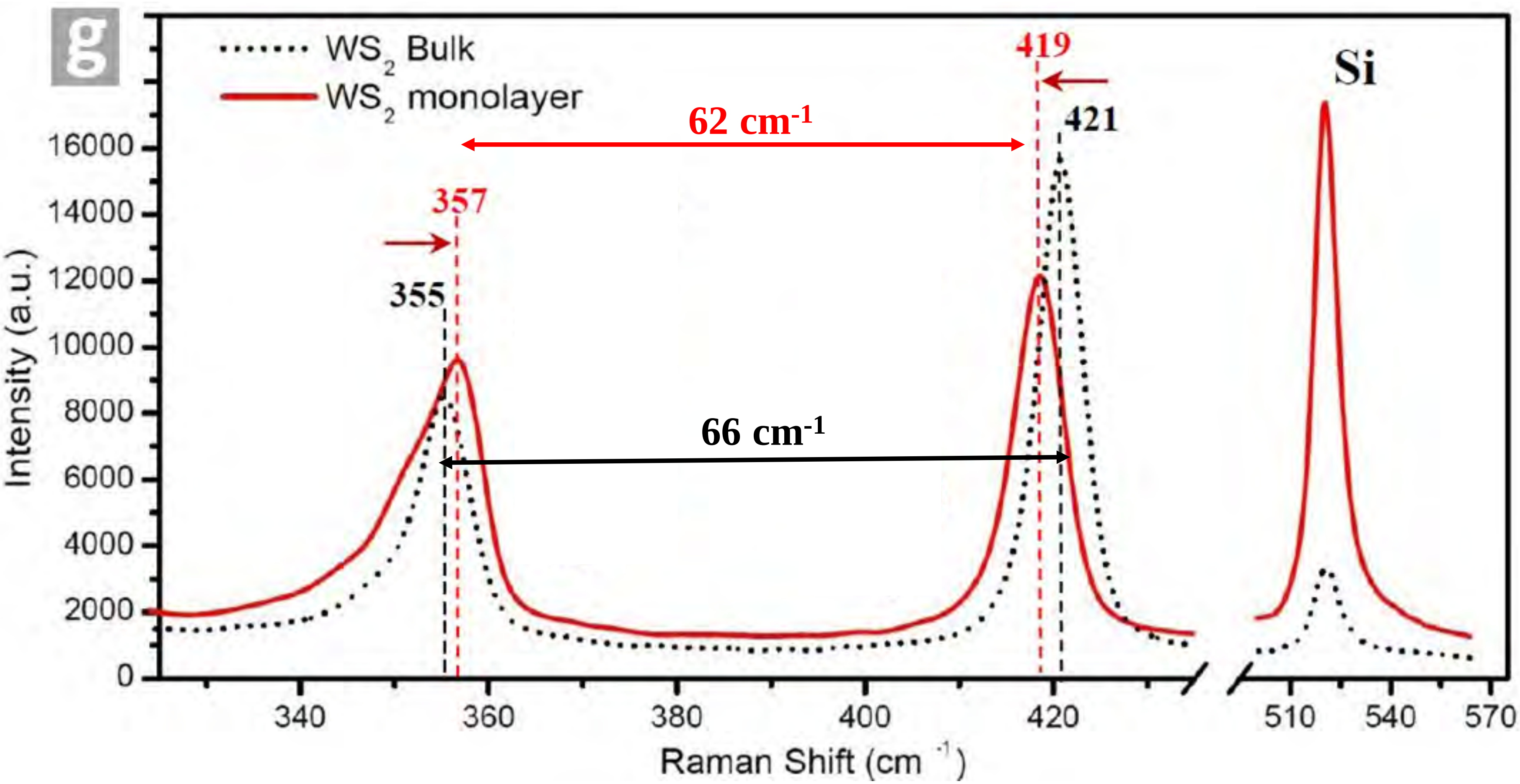




A. Berkdemir, et al. (Unpublished)

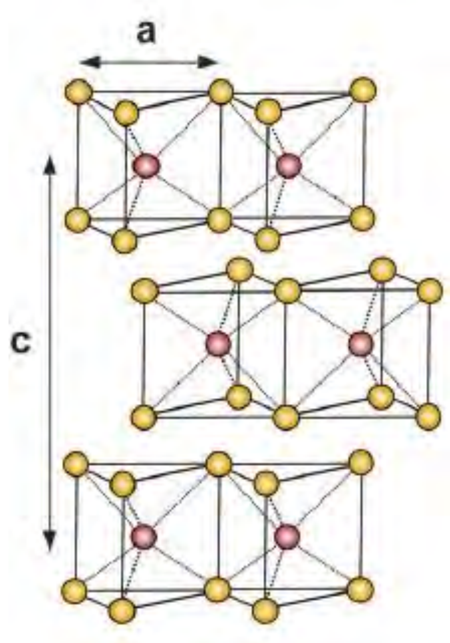
2D WS_2 islands and edge-enhanced photoluminescence

Raman Spectroscopy

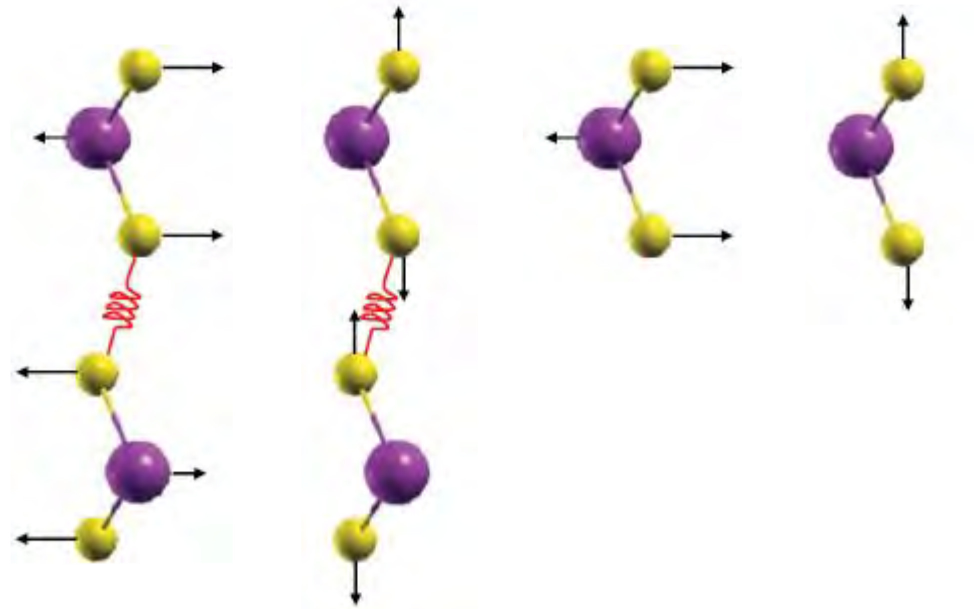


Humberto R. Gutiérrez, Nestor Perea-López, Ana Laura Elías, Ayse Berkdemir, Bei Wang, Ruitao Lv, Florentino López-Urías, Vincent H. Crespi, Humberto Terrones and Mauricio Terrones.

2-D Characterization: Raman Spectroscopy



Bulk MoS_2 in 2H phase

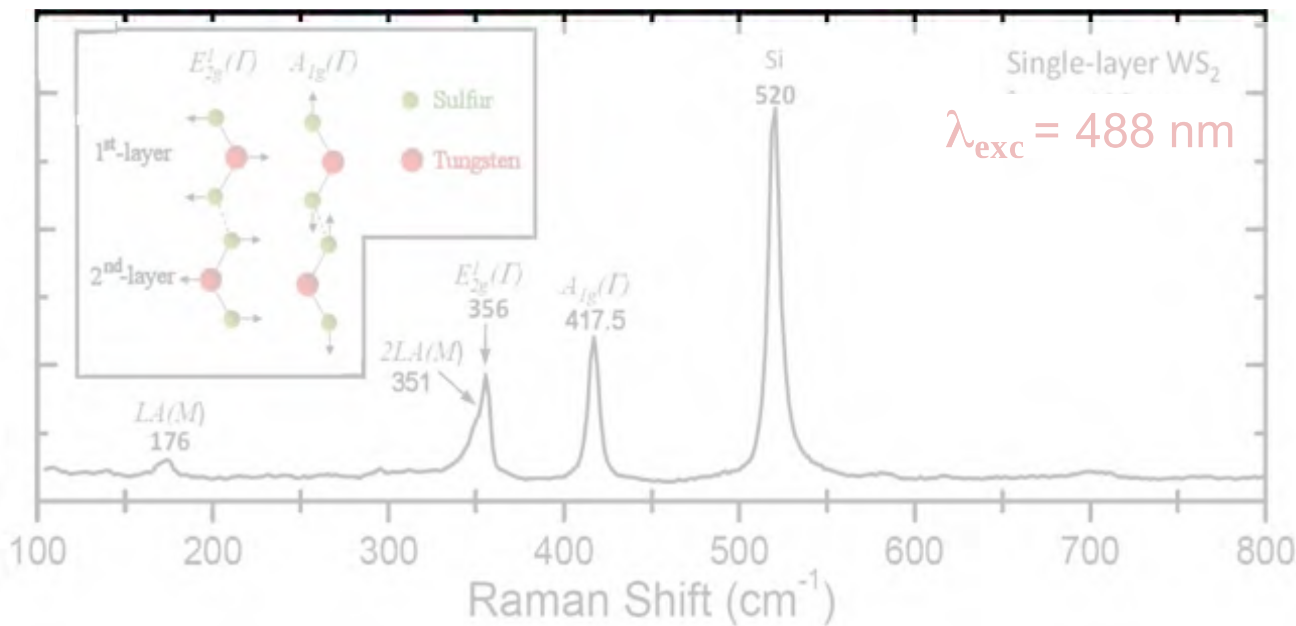


E^1_{2g} A_{1g} E' A'_1

No. of layer	Point group	Center of inversion	In plane mode	Out of plane mode
Odd	D_{3h}	No	E'	A'_1
Even	D_{3d}	Yes	E^1_{2g}	A_{1g}
Bulk	D_{6h}	Yes	E^1_{2g}	A_{1g}

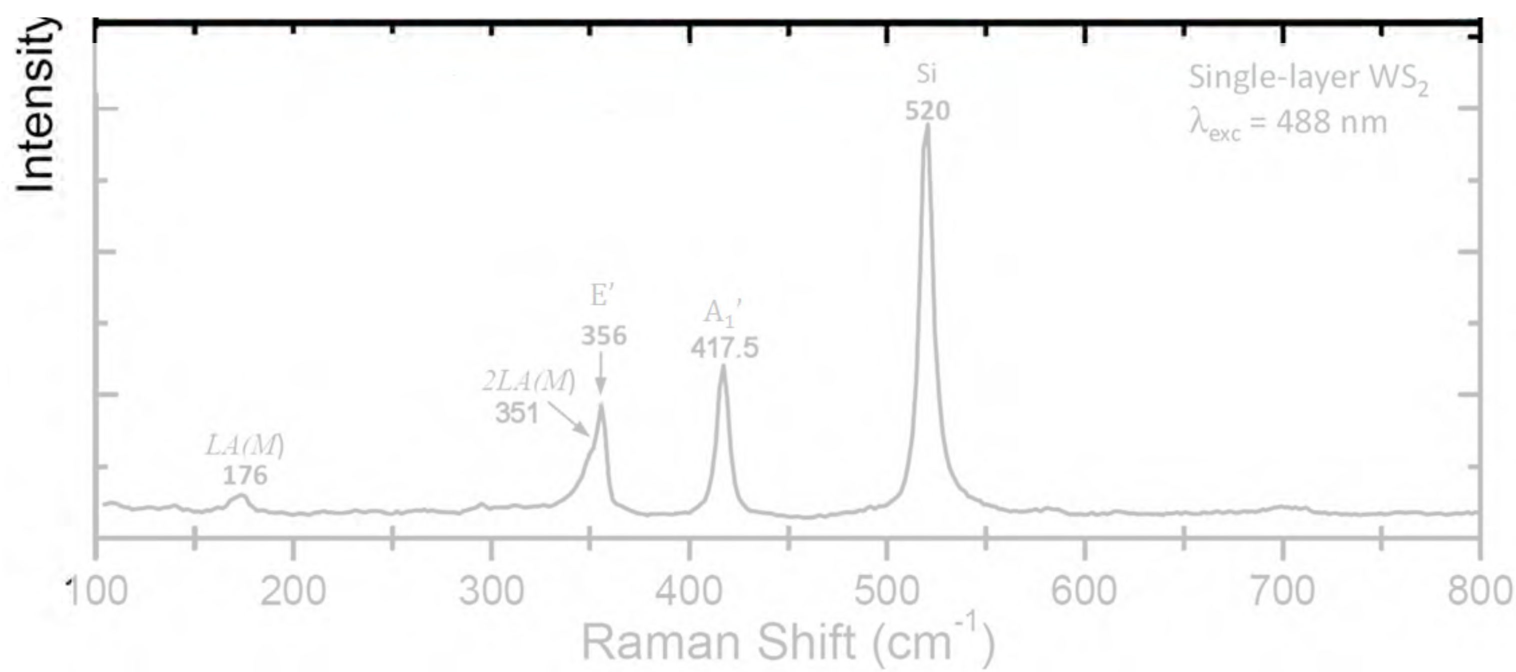
A. Molina-Sanchez, et al. Phys. Rev. B 84, 155413 (2011).
H. Terrones, et al. Sci. Rep. 4 (2014) DOI: 10.1038/srep04215.

Resonant Raman on WS_2 Monolayers



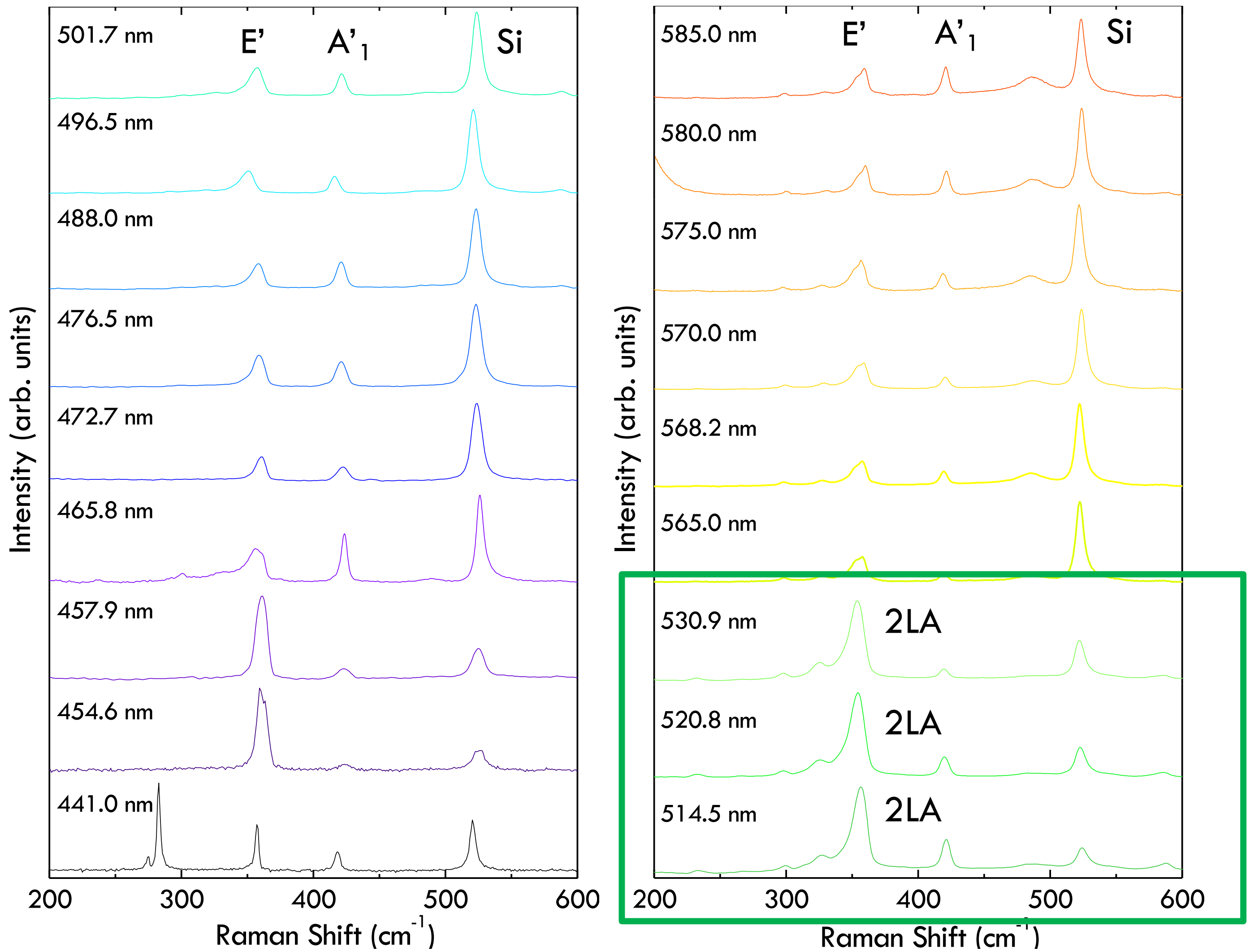
A. Berkdemir, H. R. Gutiérrez, et al. (Nature Scientific Reports 3, 1755 (2013)

Resonant Raman on WS_2 Monolayers



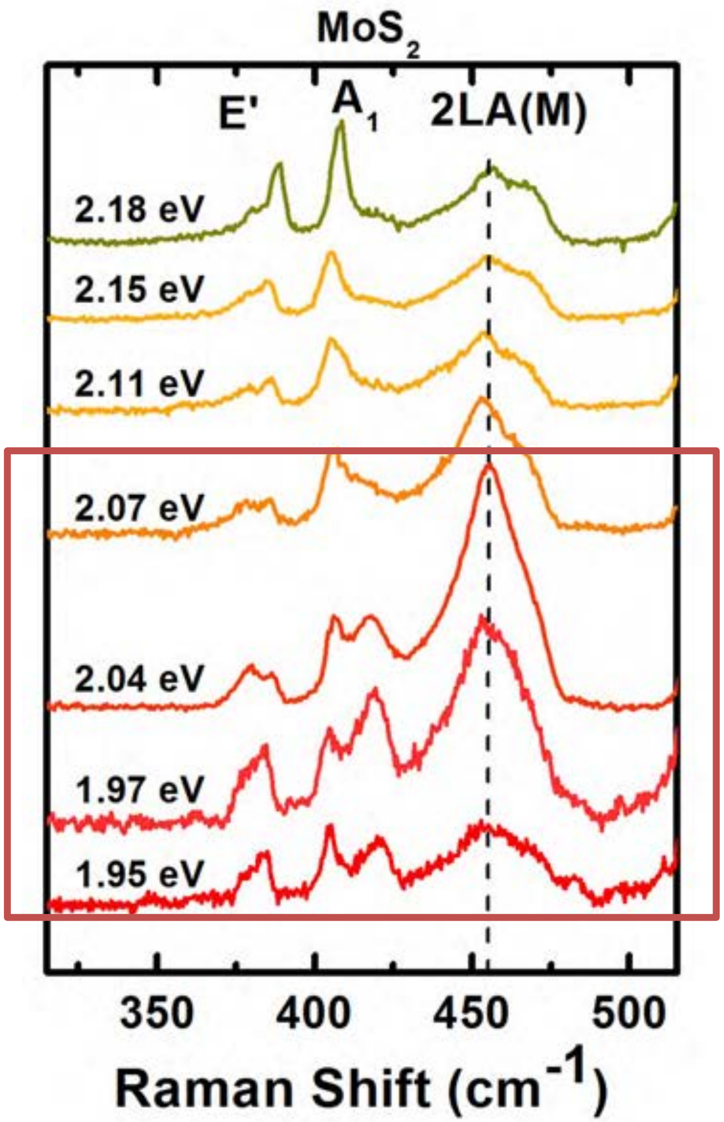
A. Berkdemir, H. R. Gutiérrez, et al. (Nature Scientific Reports 3, 1755 (2013)

Resonant Raman on WS_2 Triangular Monolayers

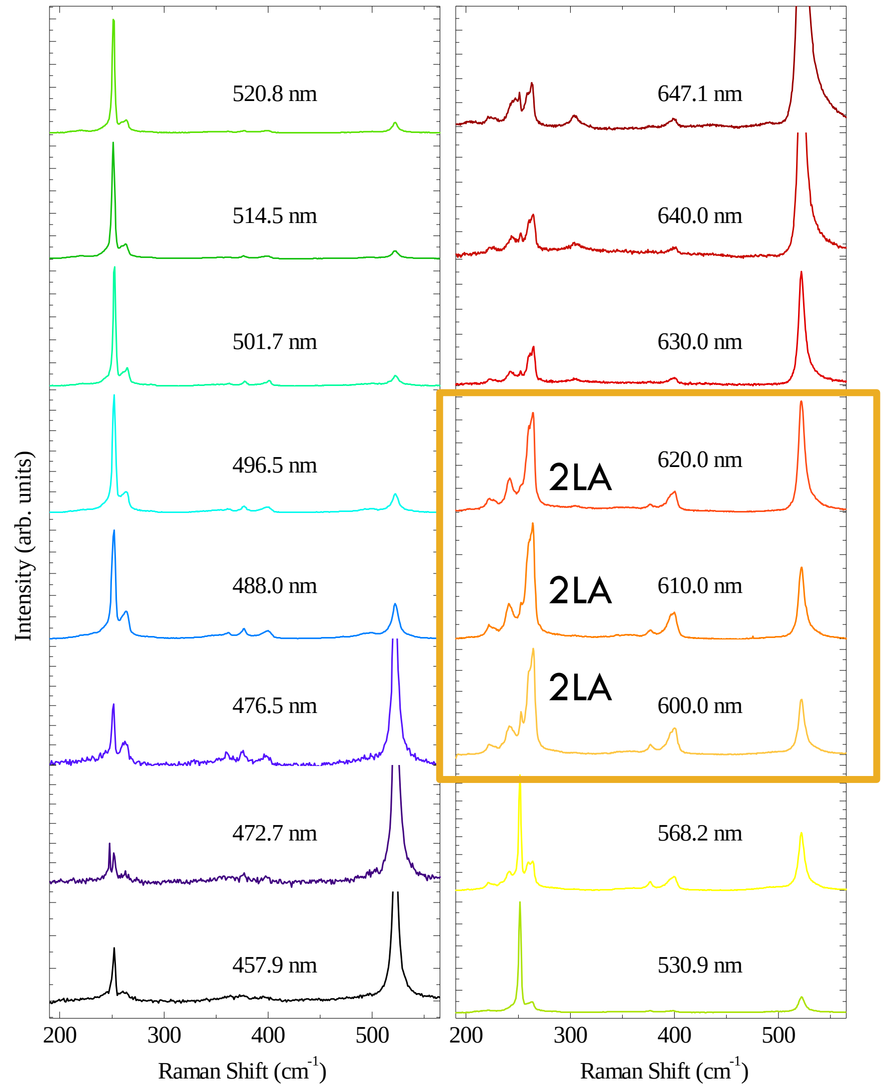


E. Del Corro, et al in preparation

Resonant Raman on MoS_2 and WSe_2 Monolayers

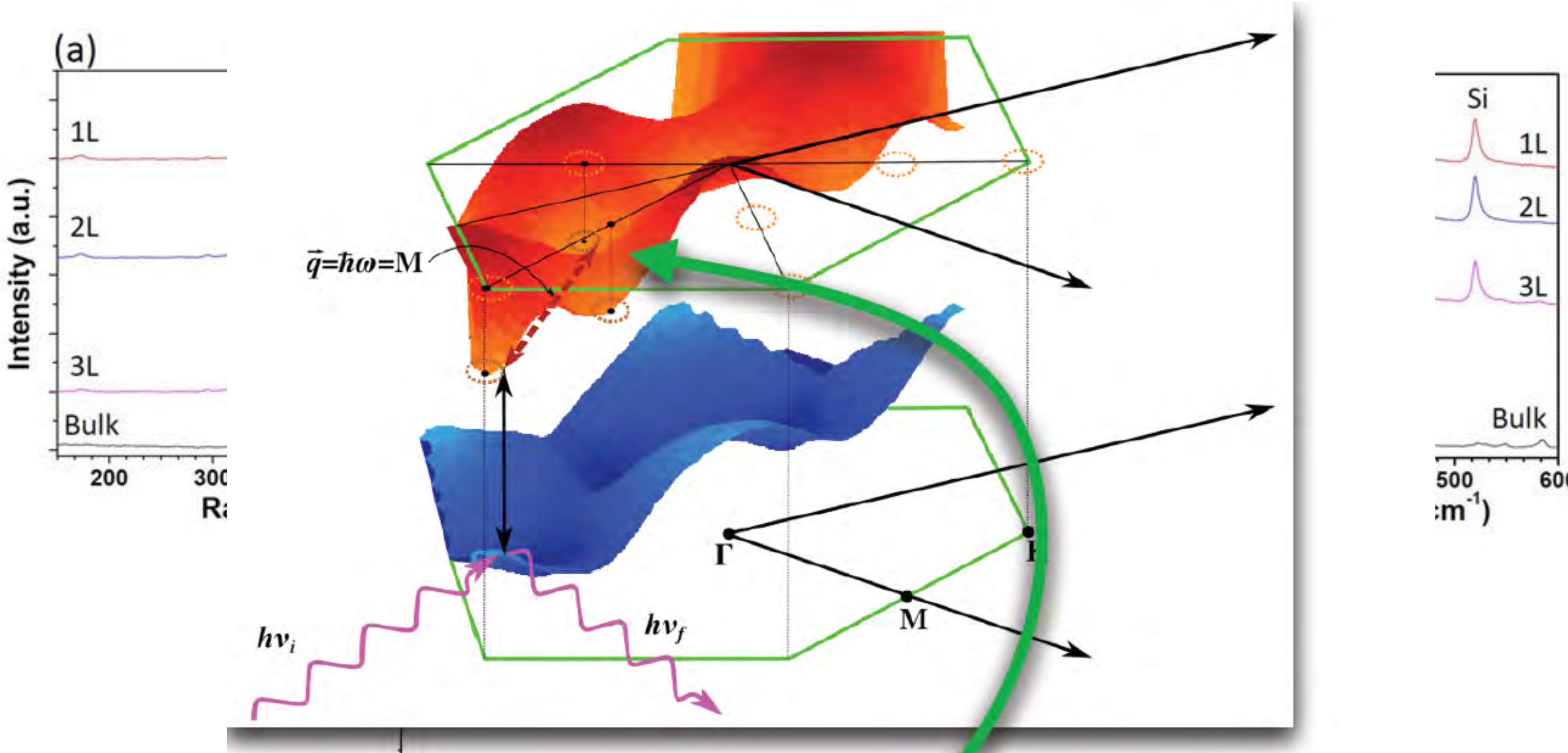


*M.A. Pimenta et al., Acc. Chem. Res., 2015, **48** (1), pp 41–47*



E. Del Corro, et al. unpublished (2015)

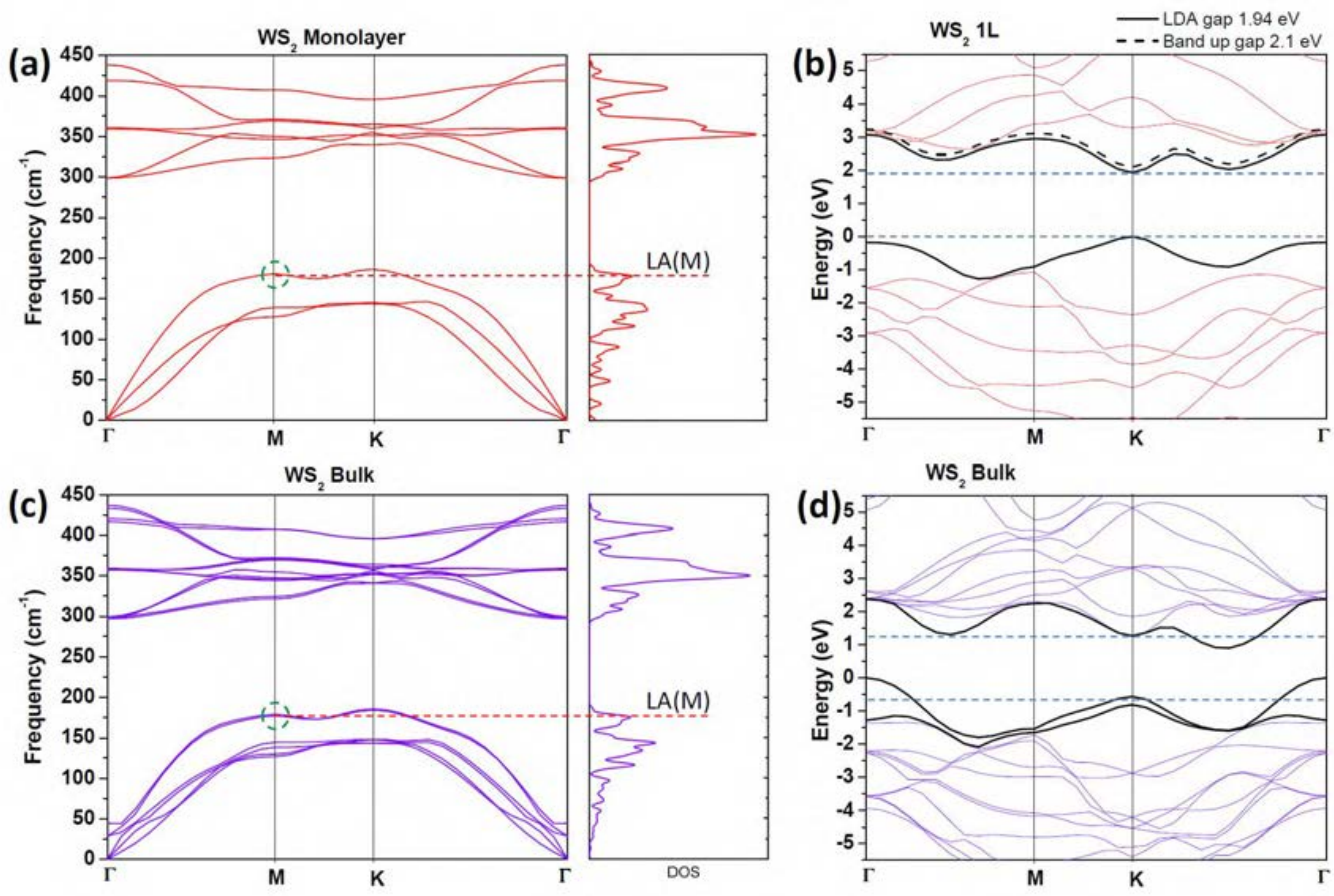
Resonant Raman on WS_2 Monolayers



This intermediate electronic state is only present in the **monolayer**. Calculation of the double resonance (for constant matrix elements) confirms the effect.

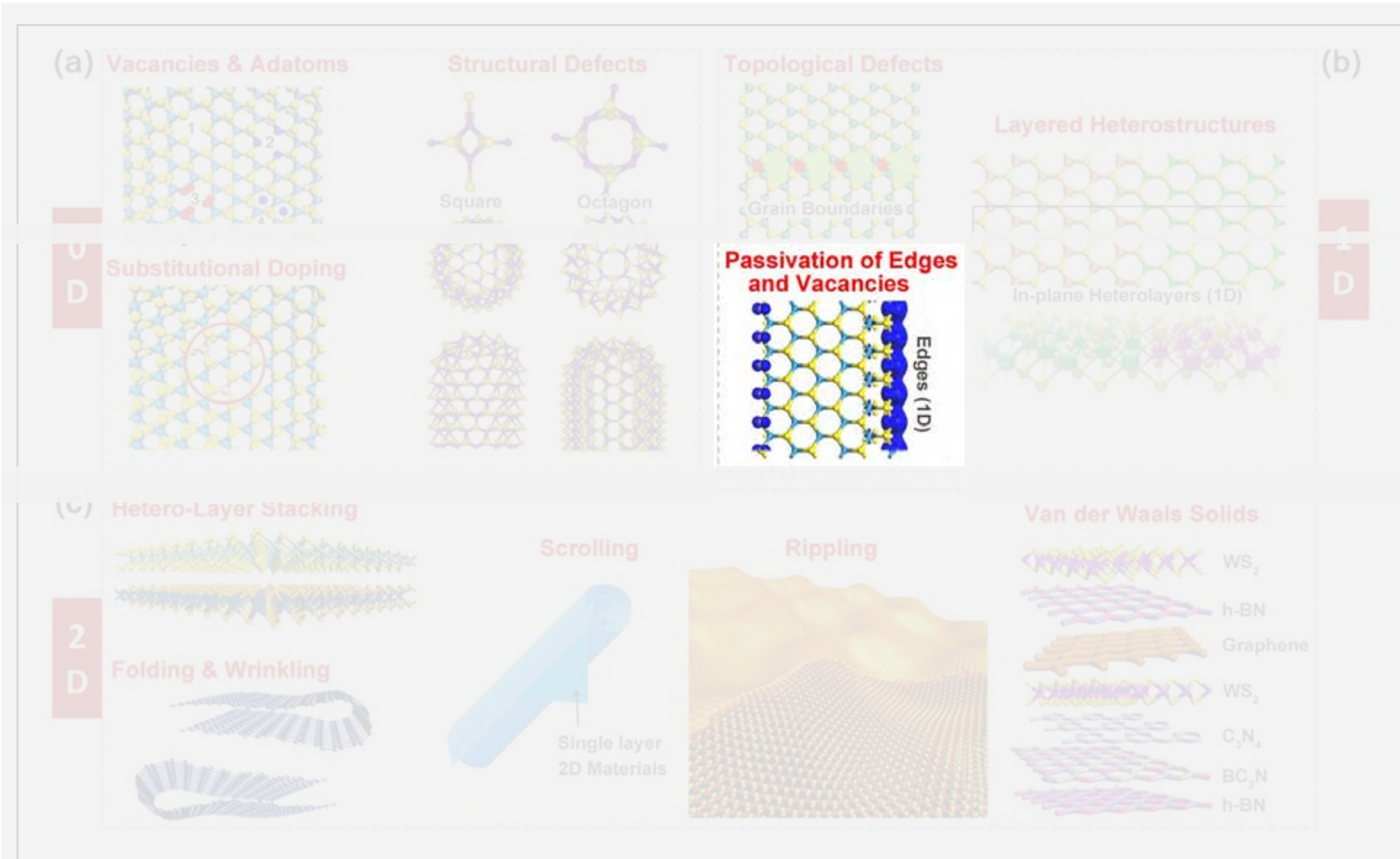
A. Berkdemir, H. R. Gutiérrez, et al. (Nature Scientific Reports 3, 1755 (2013))

Phonon dispersion and electronic band structures



A. Berkdemir, H. R. Gutiérrez, et al. (Nature Scientific Reports 3, 1755 (2013)

Defect Engineering



Z. Lin, B.R. Carvalho, E. Kahn, R. Lv, R. Rao, H. Terrones, M.A. Pimenta, M. Terrones. 2D Materials (2016)

Low Temperature Synthesis of MoS_2 & WS_2

Center for 2-Dimensional and Layered Materials Penn State

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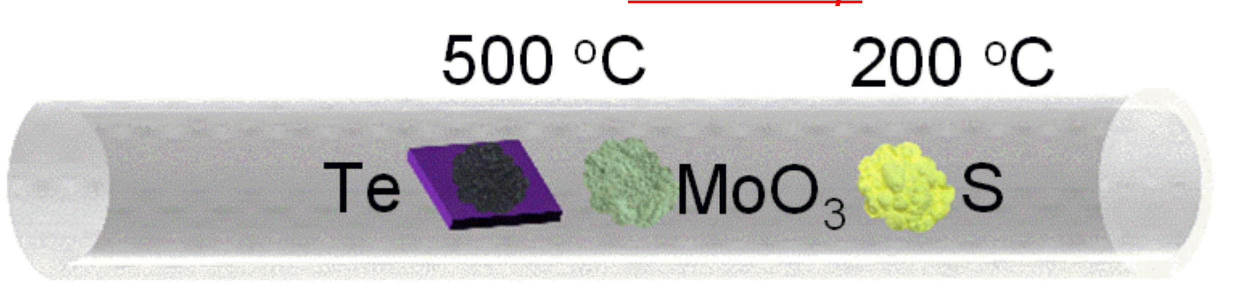
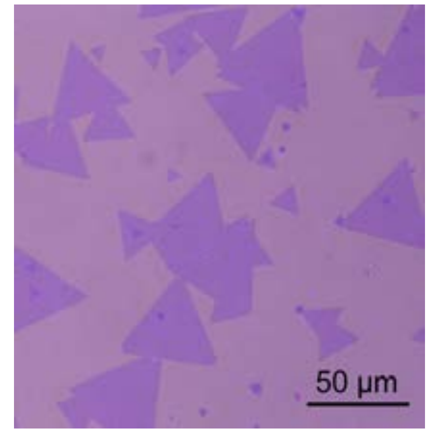
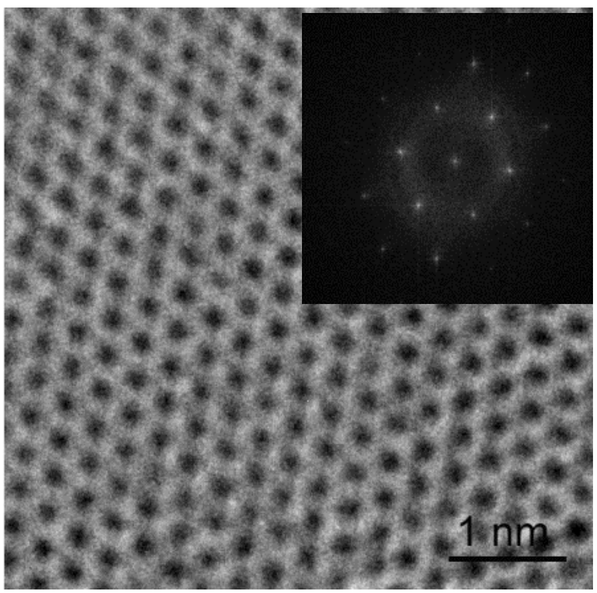
CVD setup

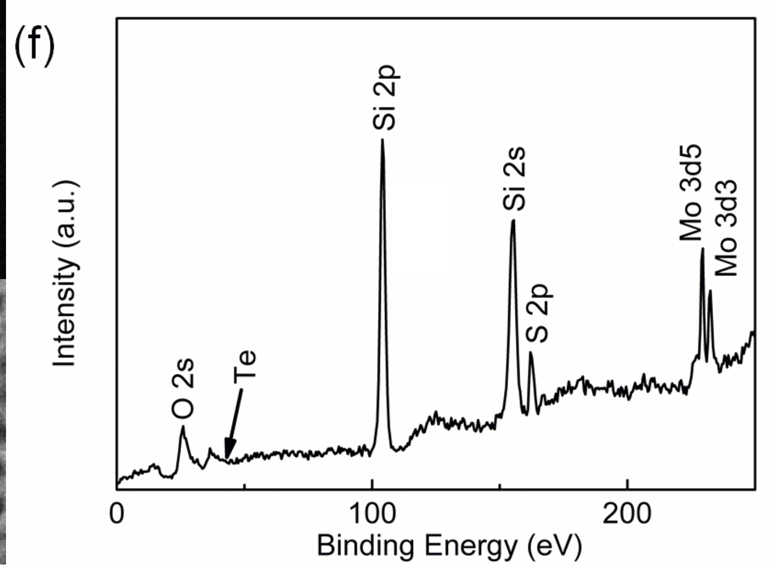


No evidence of Te doping



MoS_2 monolayers



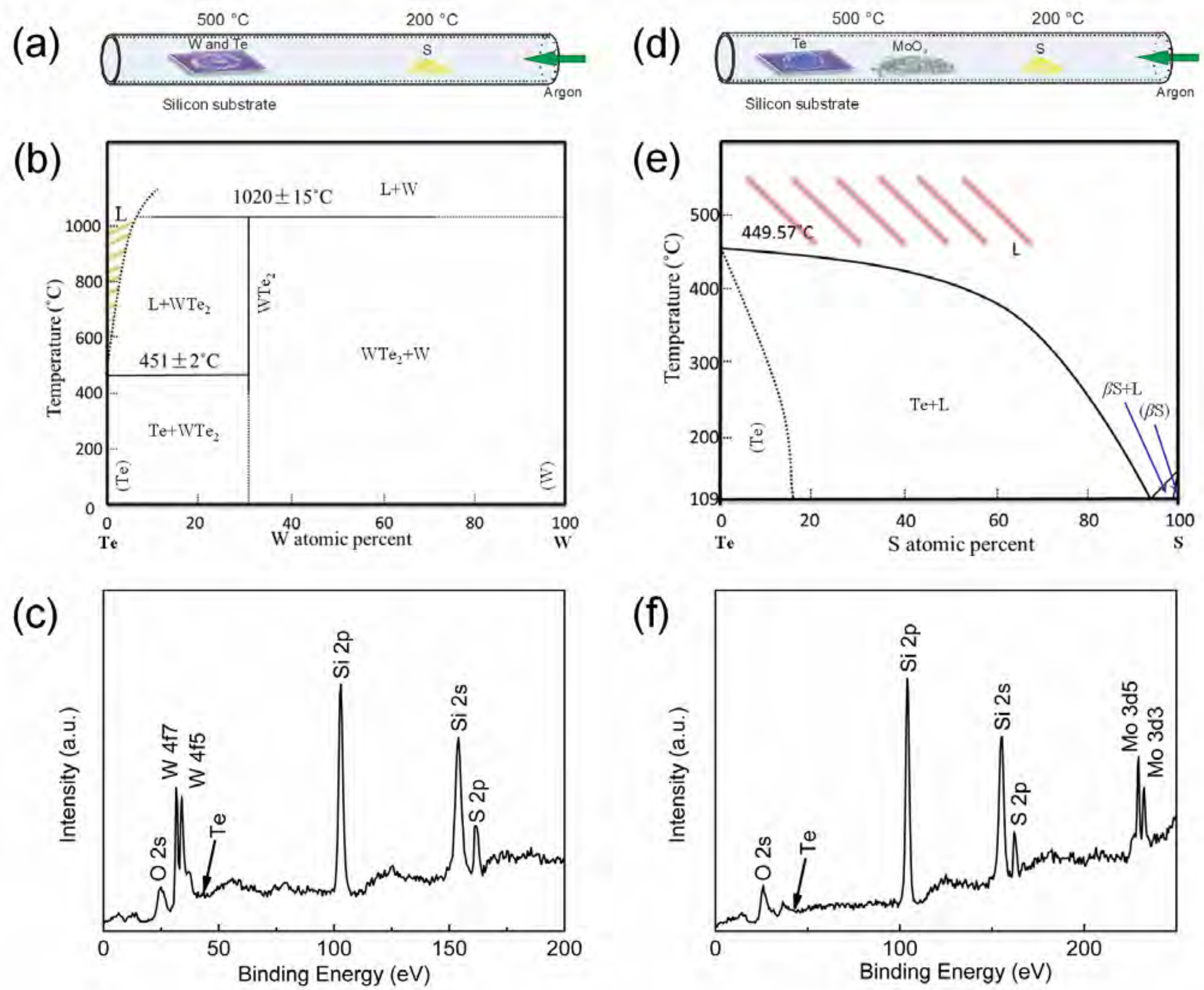


Y. Gong, Z. Lin

➢ **The presence of Te reduces the synthesis temperature**

Y. Gong, Z. Lin, P.M. Ajayan, Terrones, et al., ACS Nano (2015)

Low Temperature Synthesis of MoS_2 & WS_2



➢ **The presence of Te reduces the synthesis temperature**

Y. Gong, Z. Lin, P.M. Ajayan, Terrones, et al., unpublished (2015)

Low Temperature Synthesis of MoS_2 & WS_2

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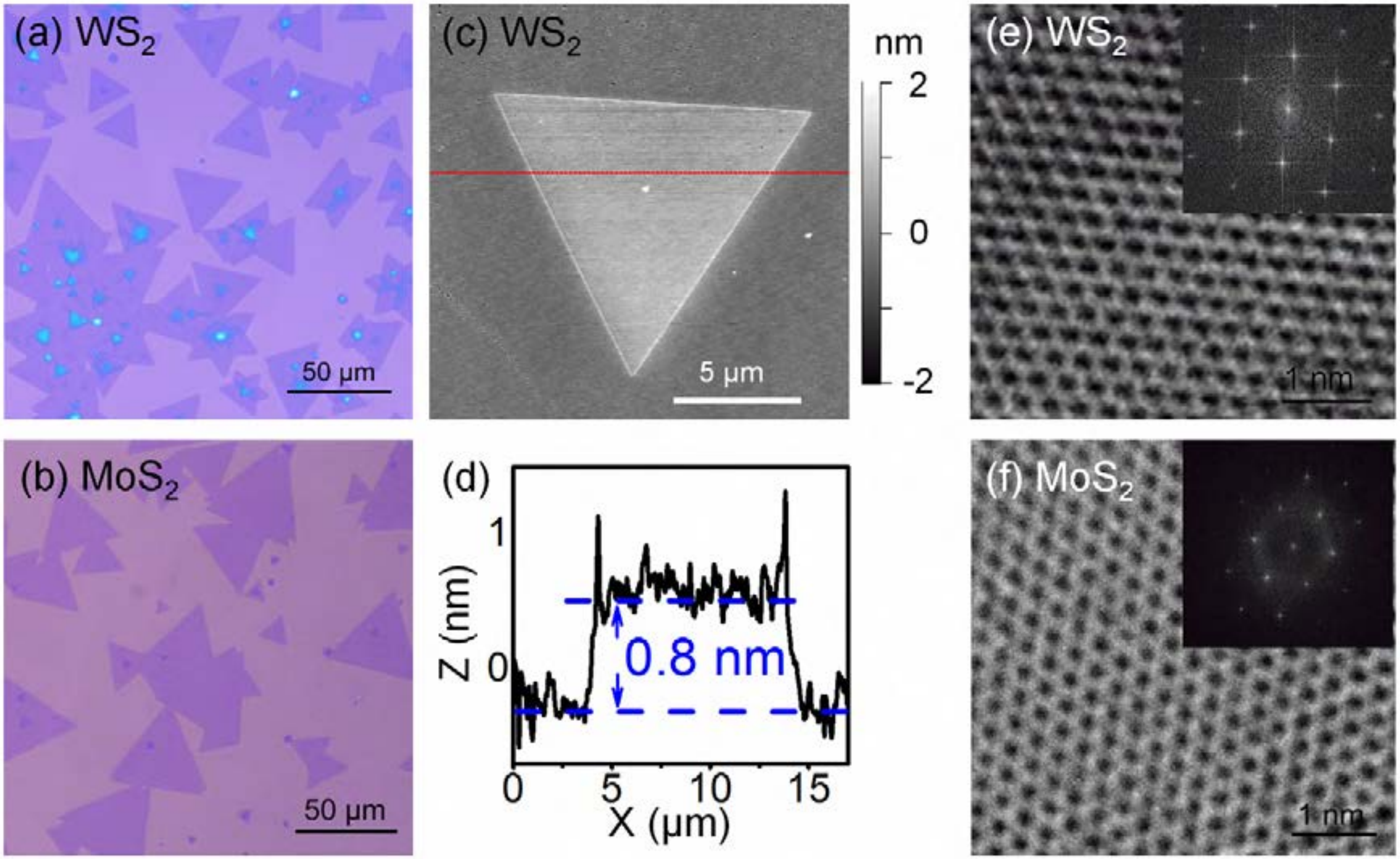

- The presence of Te reduces the synthesis temperature to 500 ºC

Y. Gong, Z. Lin, P.M. Ajayan, Terrones, et al., ACS Nano (2015)

Low Temperature Synthesis of MoS_2 & WS_2

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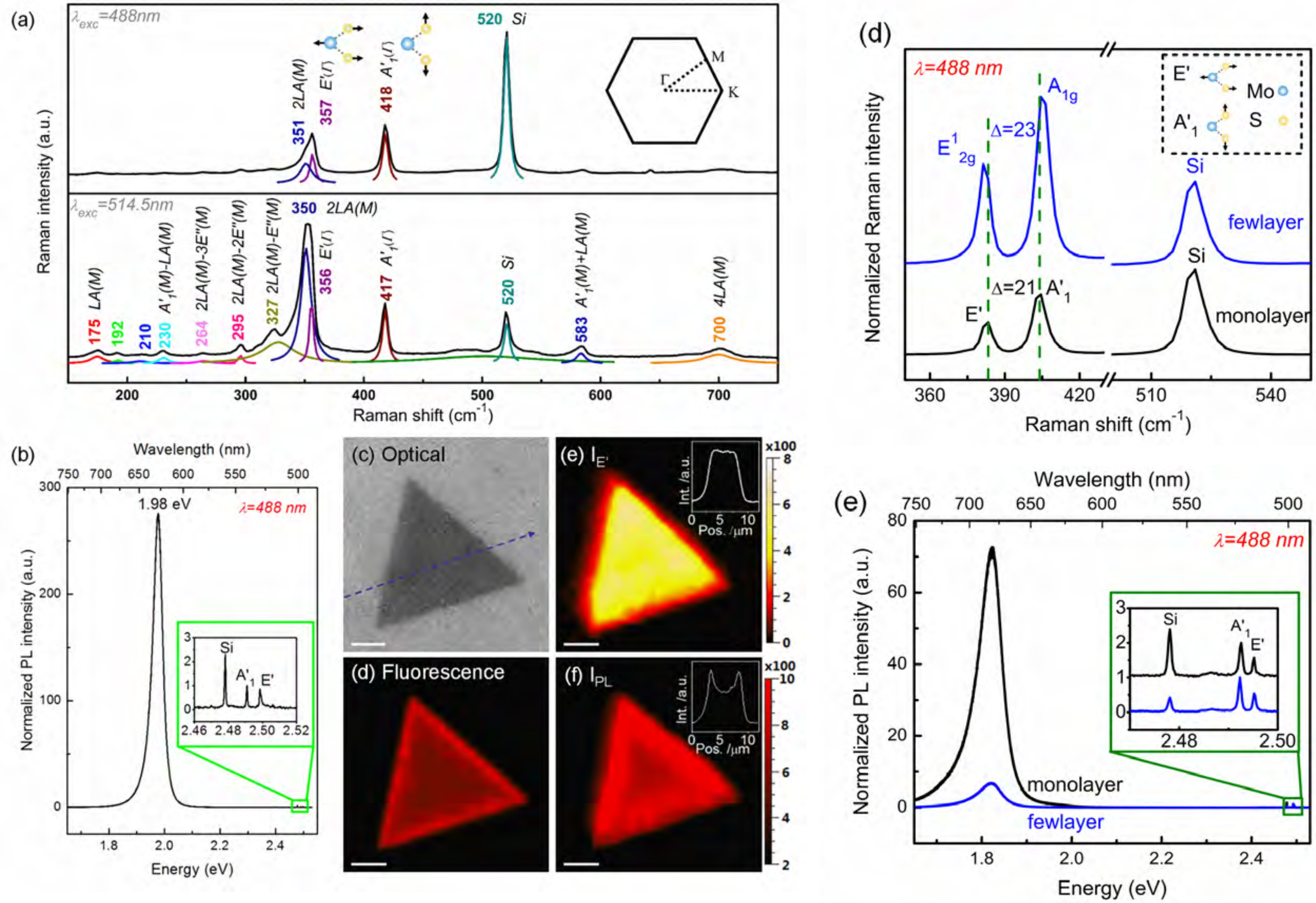
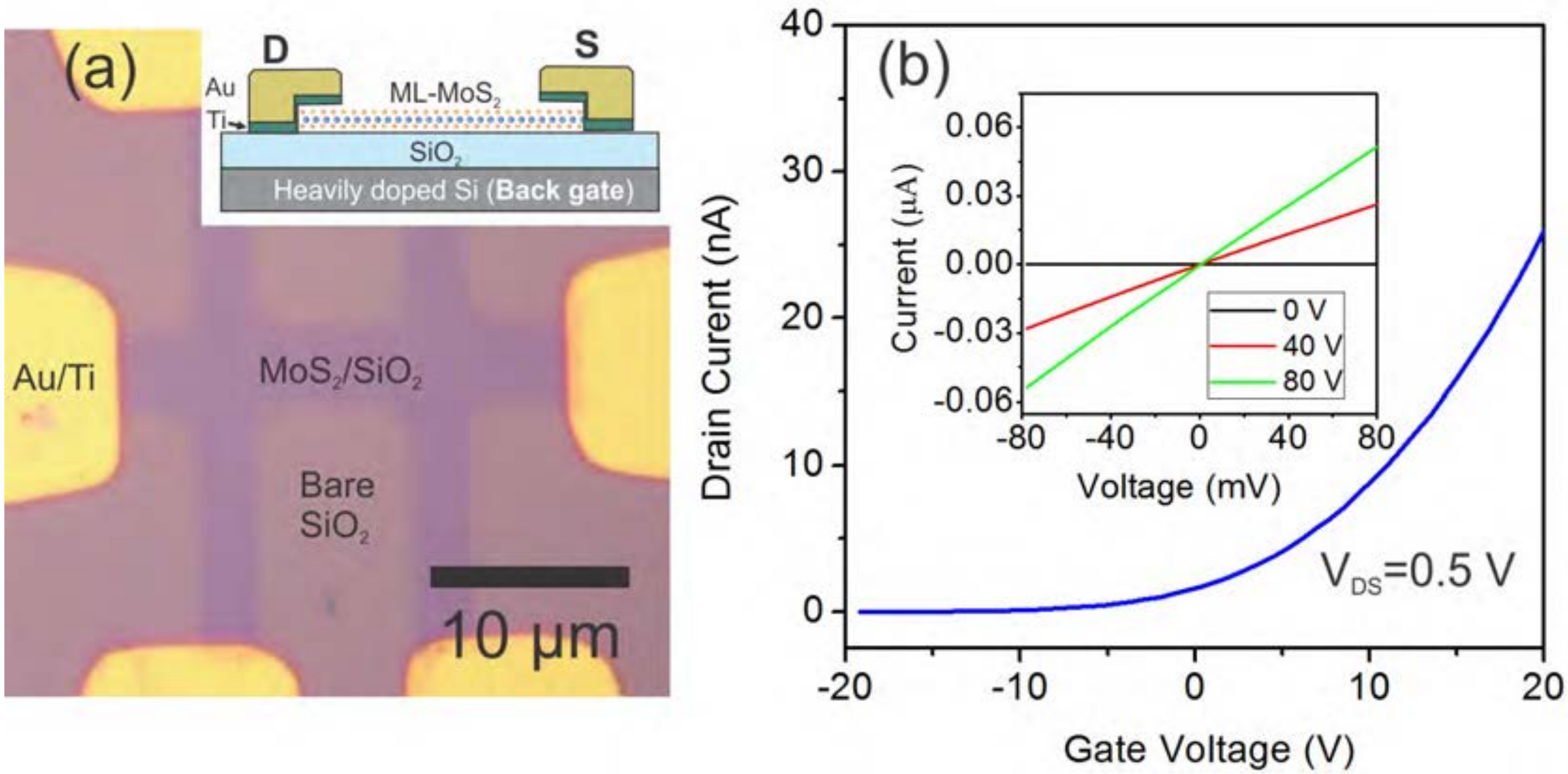


➢ **The presence of Te reduces the synthesis temperature to 500 ºC**

Y. Gong, Z. Lin, P.M. Ajayan, Terrones, et al., ACS Nano (2015)

Low Temperature Synthesis of MoS_2 & WS_2

Transport measurements reveal are very similar when compared to high temp synthesis

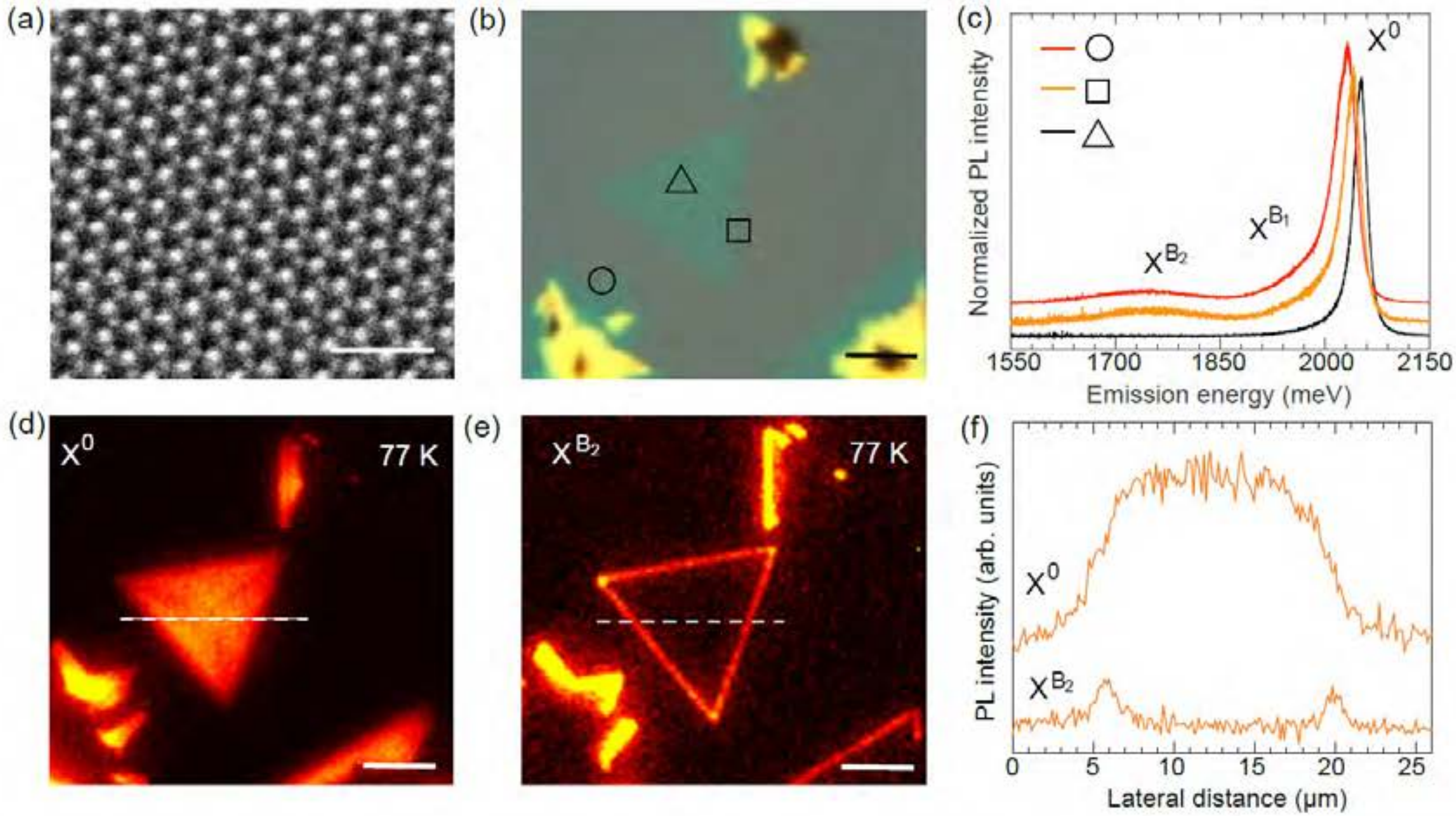


Mobility ~4.5 $cm^2V^{-2}S^{-1}$
On-off ratio ~10^5

Y. Gong, Z. Lin, P.M. Ajayan, Terrones, et al., ACS Nano (2015)

Bound Exciton Emission in Single Layer WS_2

V. Carozo, Y. Wang, et al.



(a) Atomic structure of single layer 1H-WS_2. (b) Optical image of triangular WS_2. (c) PL spectra obtained from the marked regions in (b). Photoluminescence intensity image at 77 K of (d) X^0 peak centered at 1970 meV and (e) X^B peak centered at 1690 meV. (f) X^B and X^B intensity profile acquired along the dashed line in (d) and (e).

V. Carozo, Y. Wang, V, Crespi, M. Terrones, et al., unpublished (2016)

Bound Exciton Emission in Single Layer WS_2

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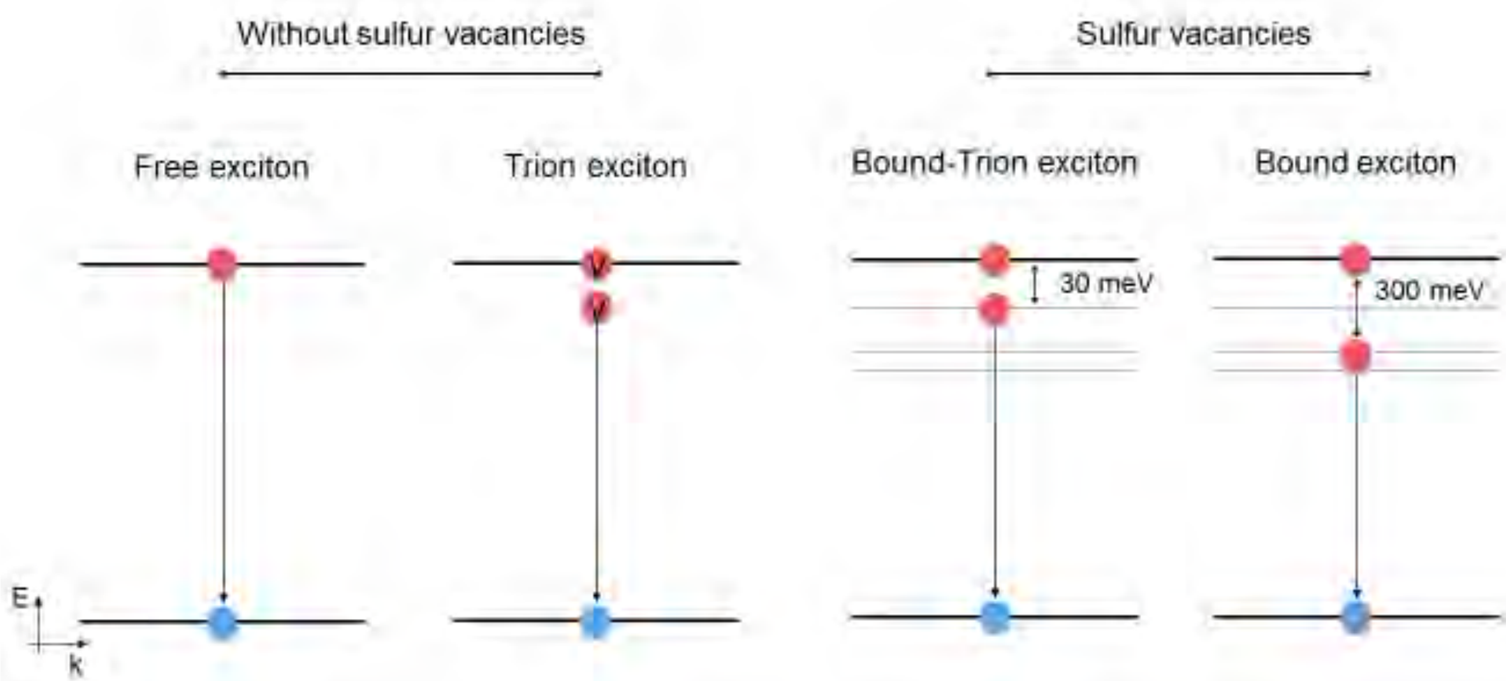

V. Carozo, Y. Wang

Bound Exciton Emission in Single Layer WS_2

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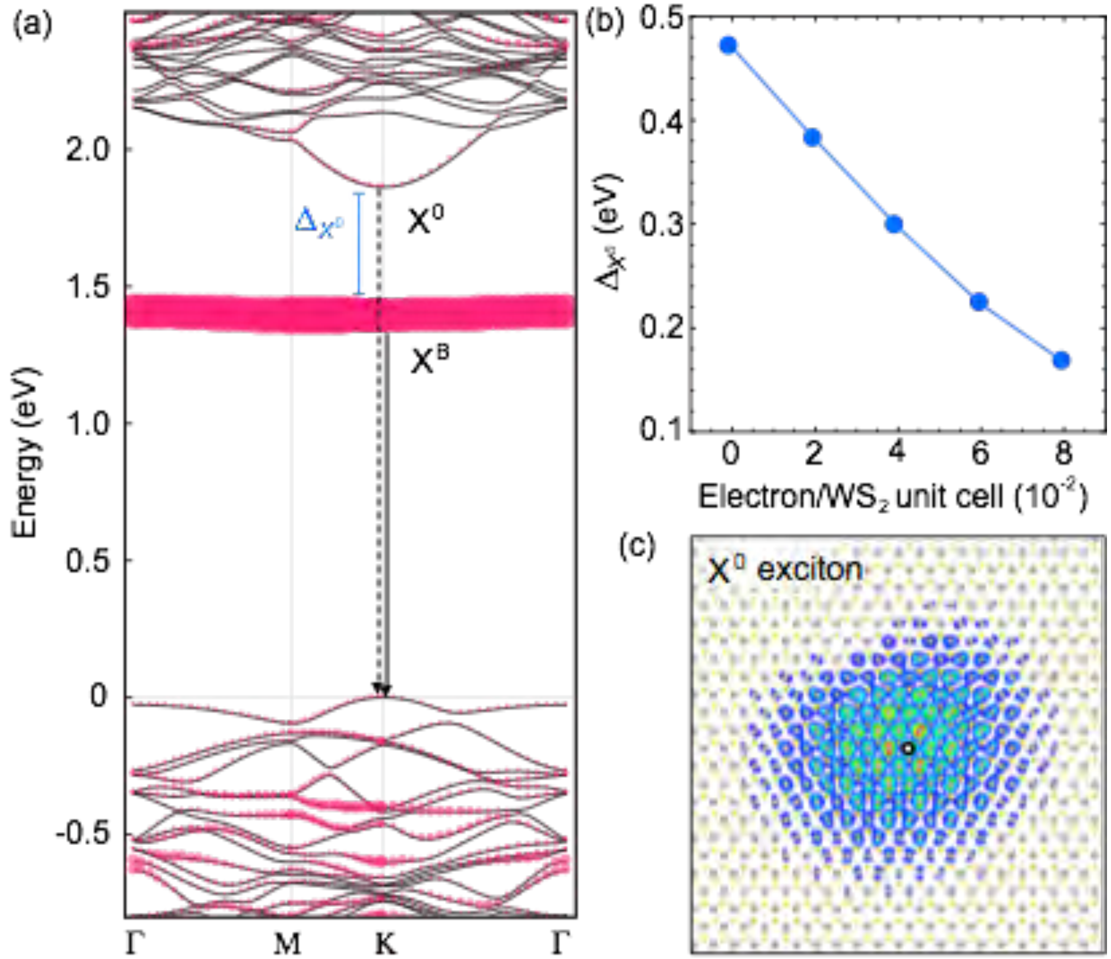

V. Carozo, Y. Wang

(a) Band structure of 5×5 WS_2 supercell containing a single sulfur vacancy. (b) The energy difference between the defect state and the conduction band minimum X^B as a function of the density of extra electrons added to the system. (c) The modulus square of the X^0 exciton wavefunction in real space

V. Carozo, Y. Wang, V, Crespi, M. Terrones, et al., unpublished (2016)

Bound Exciton Emission in Single Layer WS_2

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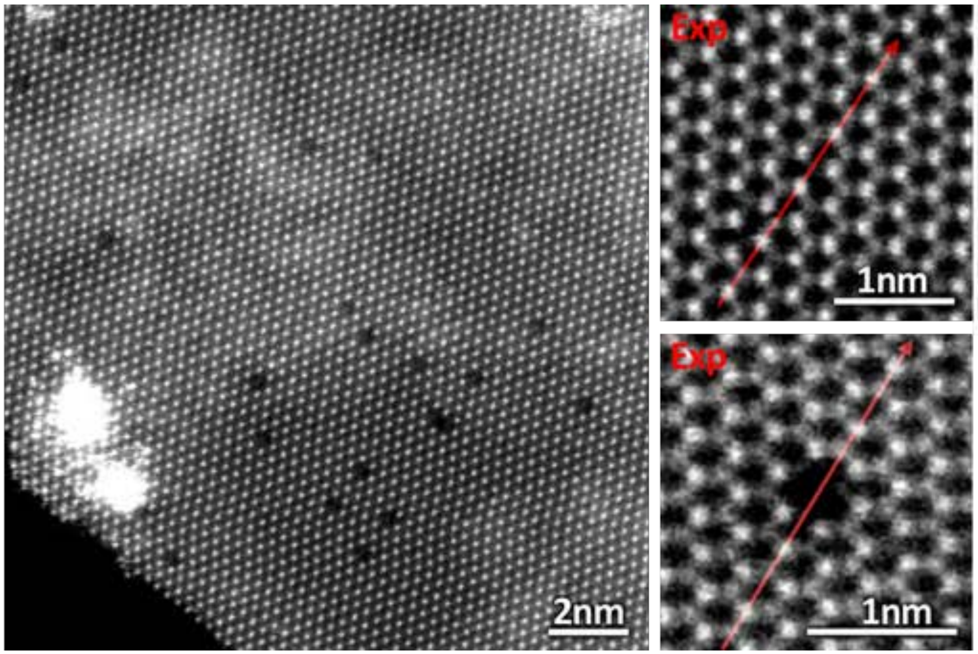
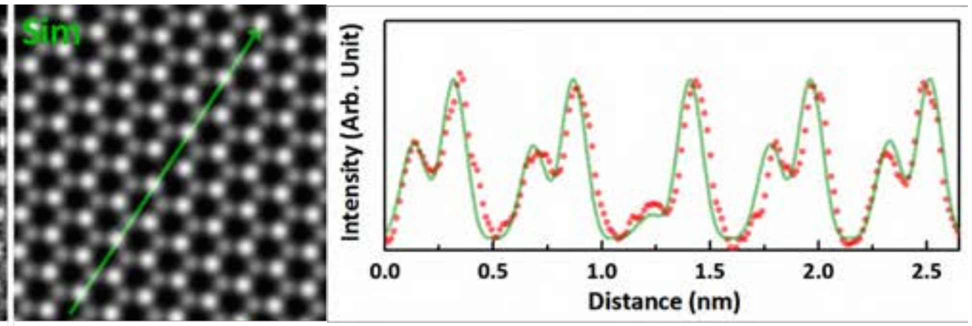
Vacancies found at edges (as-synthesized samples)





- **Challenges remaining**

Why edges have more concentration of point defects?

Is it possible to anneal defects and remove the bound exciton peak?

V. Carozo, Y. Wang, V, Crespi, M. Terrones, et al., unpublished (2016)

Growing MoS_2 Hydrophobic Nanoflowers

Center for 2-Dimensional and Layered Materials Penn State

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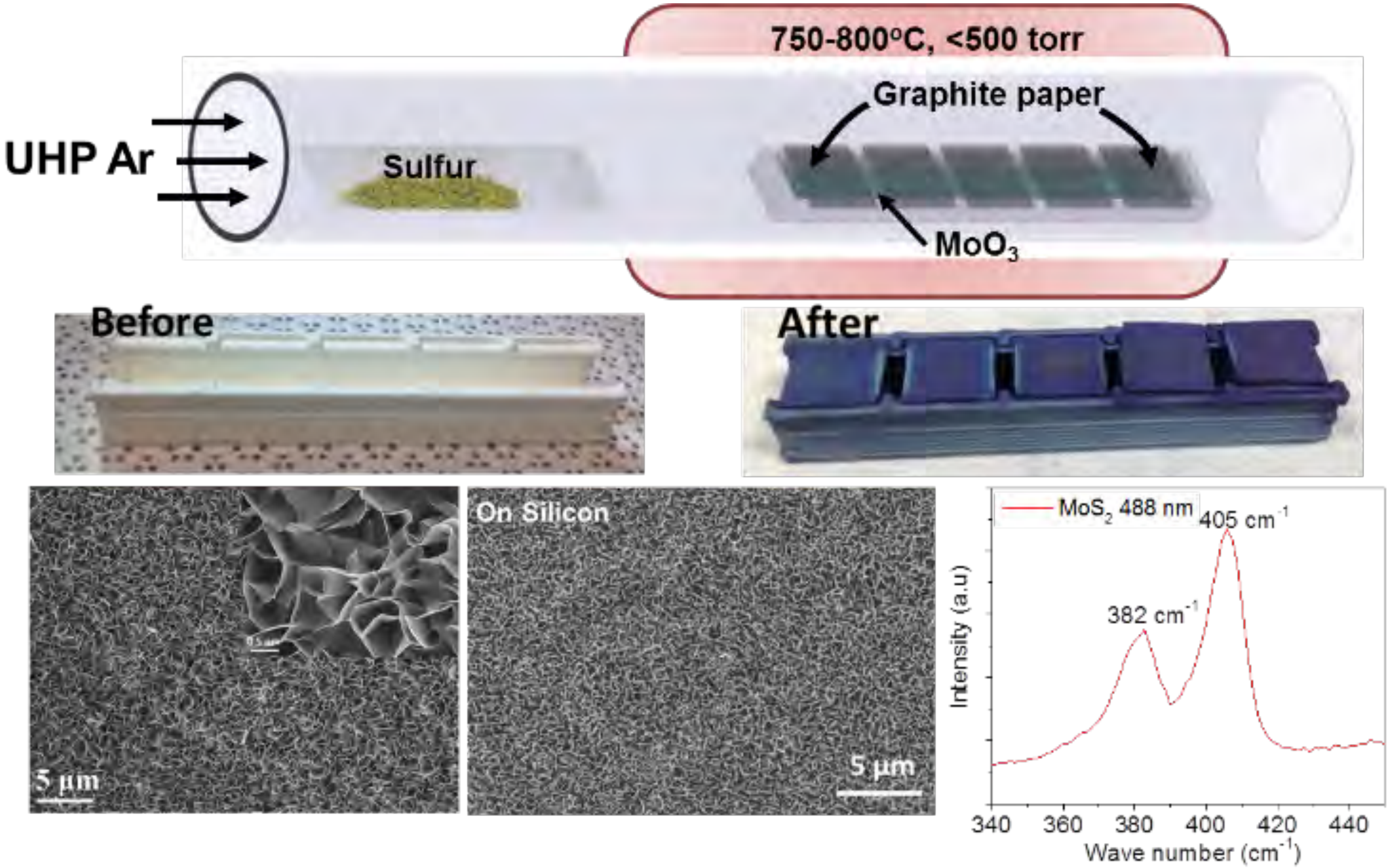
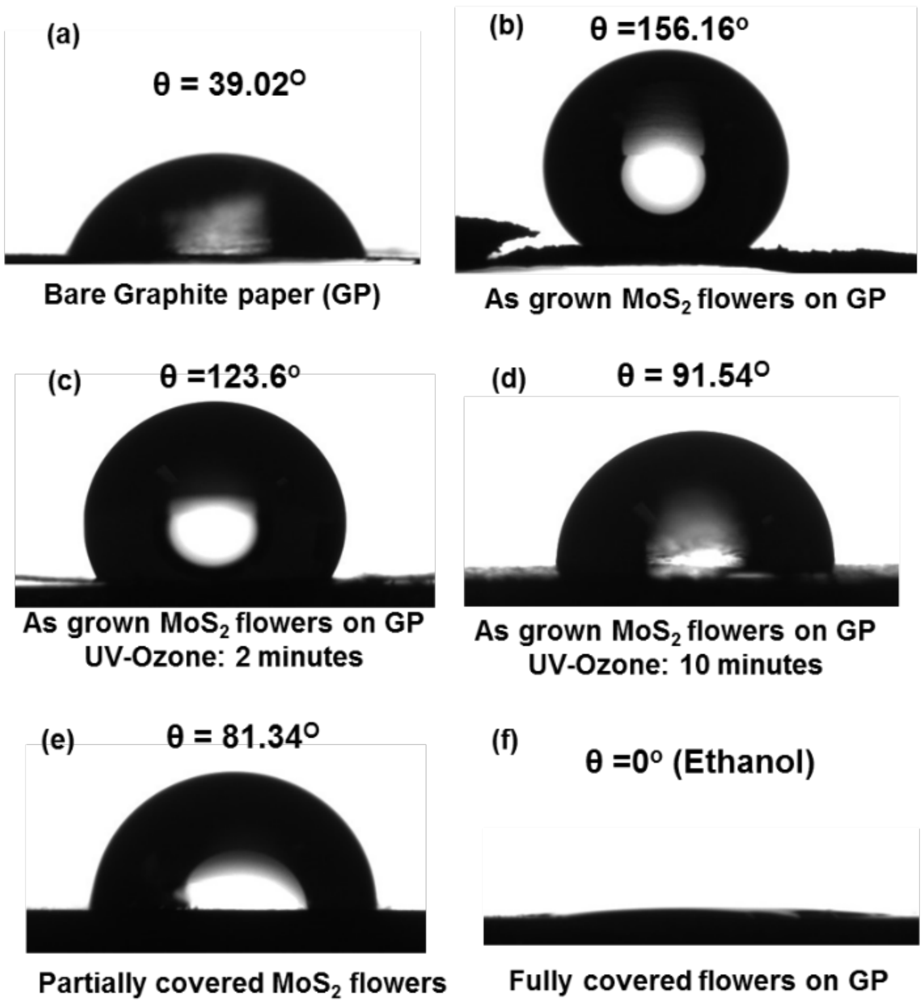
In collaboration with Robinson's Group

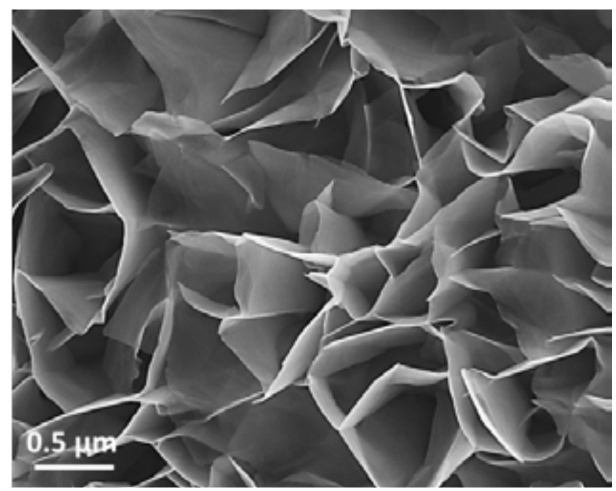


G.R Bhimanapati, Y. Lei, M. Terrones, J.A. Robinson et al., submitted (2016)

Growing MoS_2 Hydrophobic Nanoflowers

In collaboration with Robinson's Group





G.R Bhimanapati, Y. Lei, M. Terrones, J.A. Robinson et al., submitted (2016)

HER of MoS_2 Hydrophobic Nanoflowers

Center for 2-Dimensional and Layered Materials Penn State

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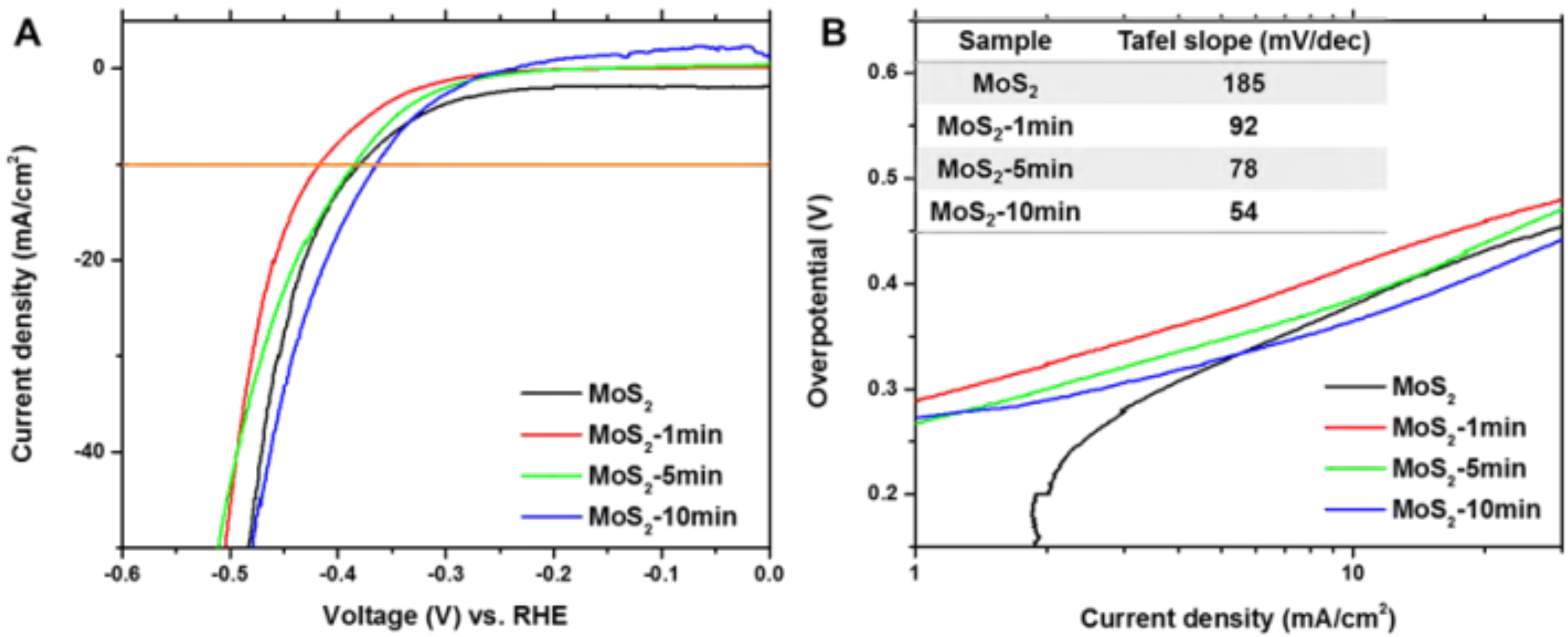
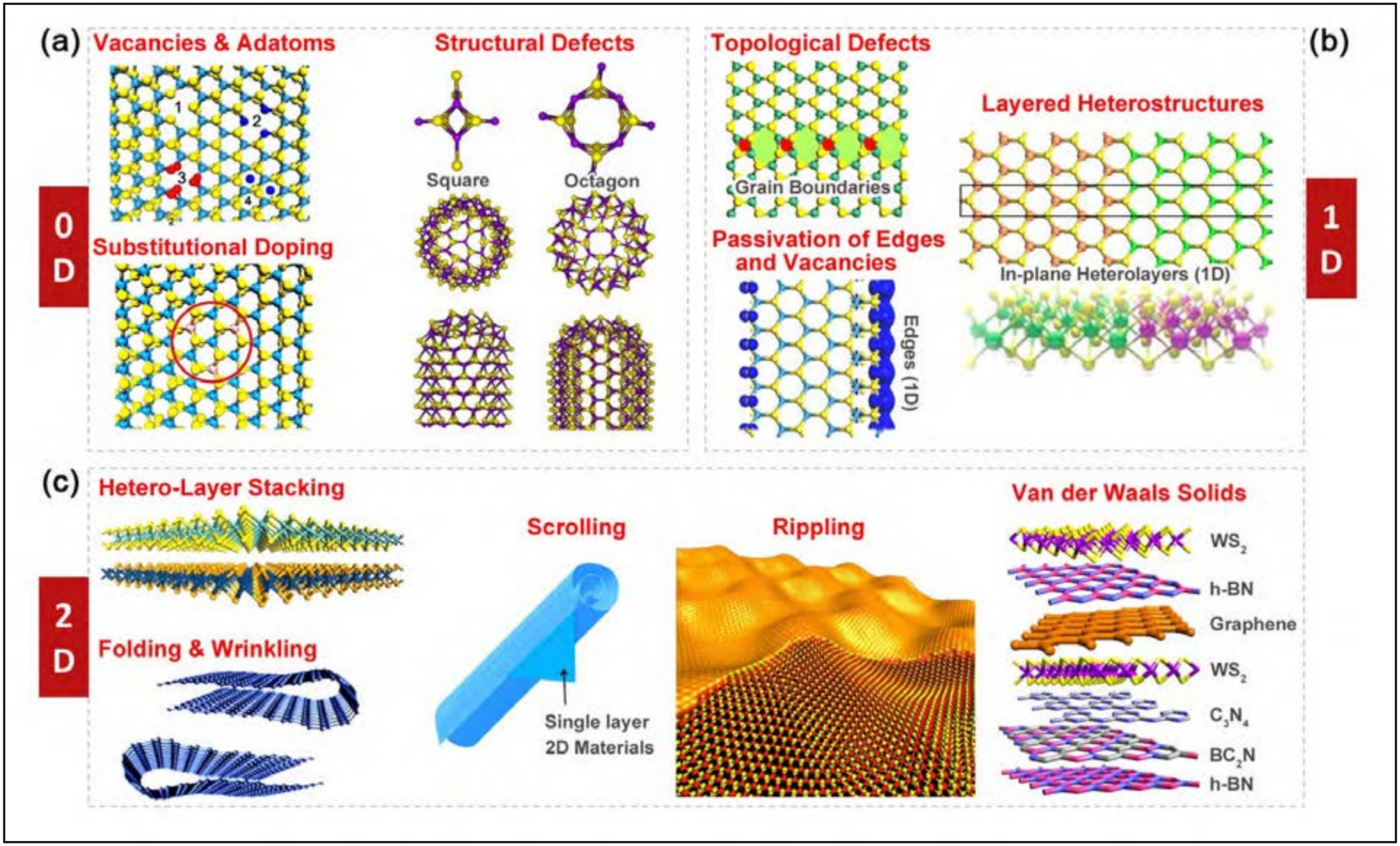
In collaboration with Robinson's Group



(a) Polarization curves of MoS_2 with different ozone treatment time (1 min, 5 min, and 10 min); and (b) the corresponding Tafel slopes, the inset table are the fitted Tafel slopes.

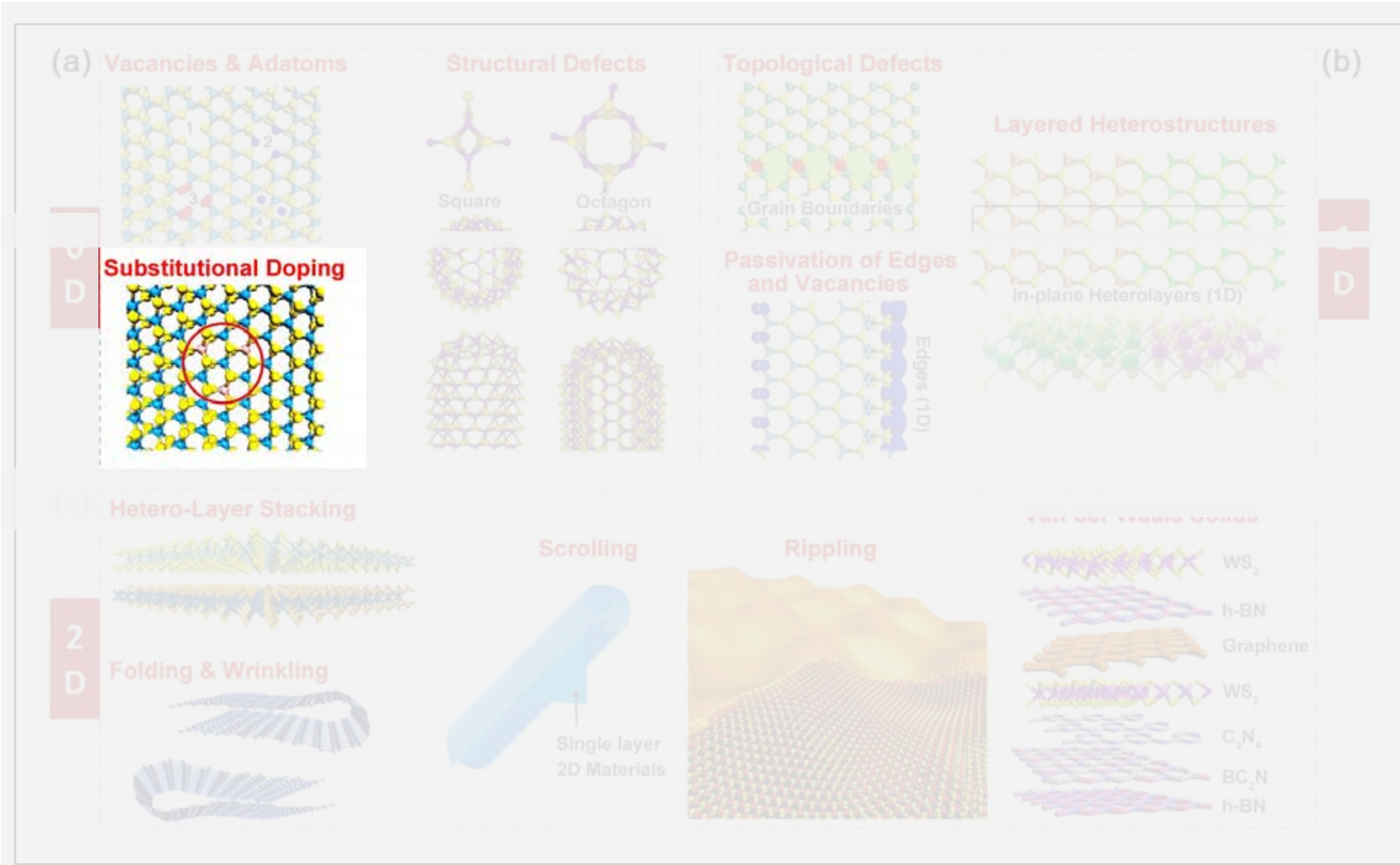
G.R Bhimanapati, Y. Lei, M. Terrones, J.A. Robinson et al., submitted (2016)

Defect Engineering



Z. Lin, B.R. Carvalho, E. Kahn, R. Lv, R. Rao, H. Terrones, M.A. Pimenta, M. Terrones. 2D Materials (2016)

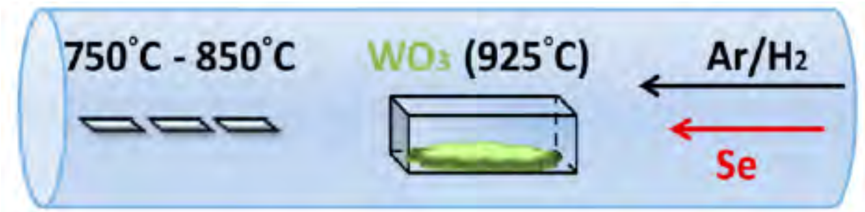
Defect Engineering



Z. Lin, B.R. Carvalho, E. Kahn, R. Lv, R. Rao, H. Terrones, M.A. Pimenta, M. Terrones. 2D Materials (2016)

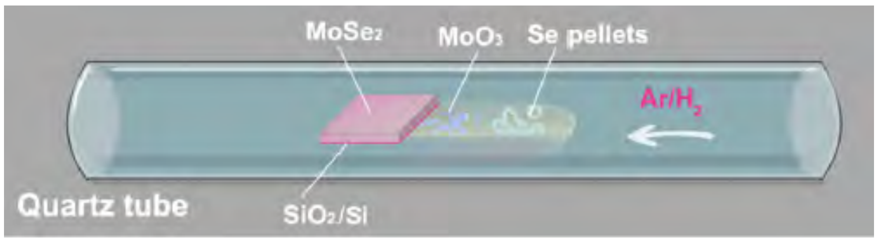
Synthesis of 2D transition metal diselenide

----from single phase to alloy



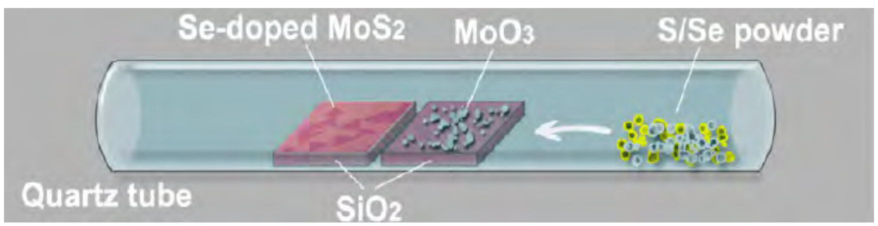
$$WO_3 + Se + H_2 \rightarrow WSe_2$$

Huang, et al. ACS Nano 8 (2014) 923.



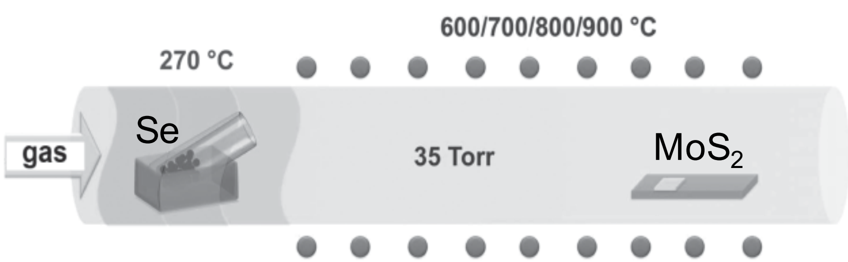
$$MoO_3 + Se + H_2 \rightarrow MoSe_2$$

Wang, et al. ACS Nano 8 (2014) 5125.



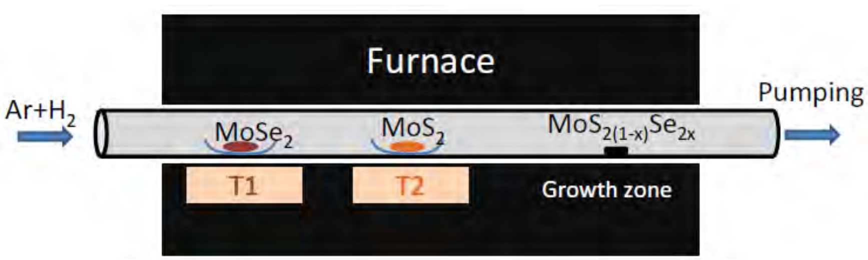
$$MoO_3 + Se + S \rightarrow MoS_xSe_{2-x}$$

Gong, et al. Nano Lett. 14 (2014) 442.



$$MoS_2 + Se \rightarrow MoS_xSe_{2-x}$$

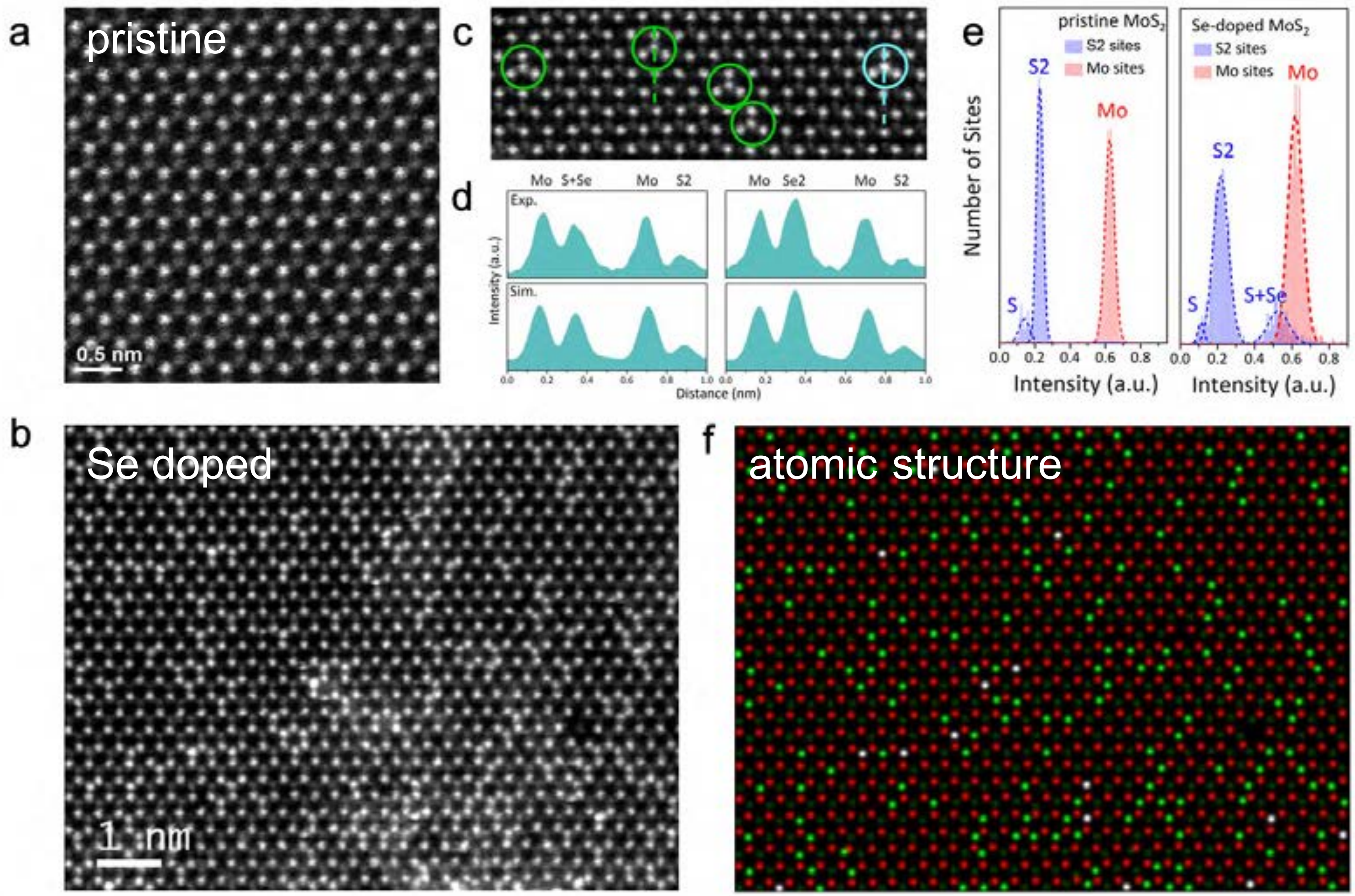
Su, et al. Small 10 (2014) 2589.



$$MoS_2 + MoSe_2 + H_2 \rightarrow MoS_xSe_{2-x}$$

Feng, et al. Adv. Mater. 26 (2014) 2648.

Dopant analysis of $MoS_{2(1-x)}Se_{2x}$ monolayer

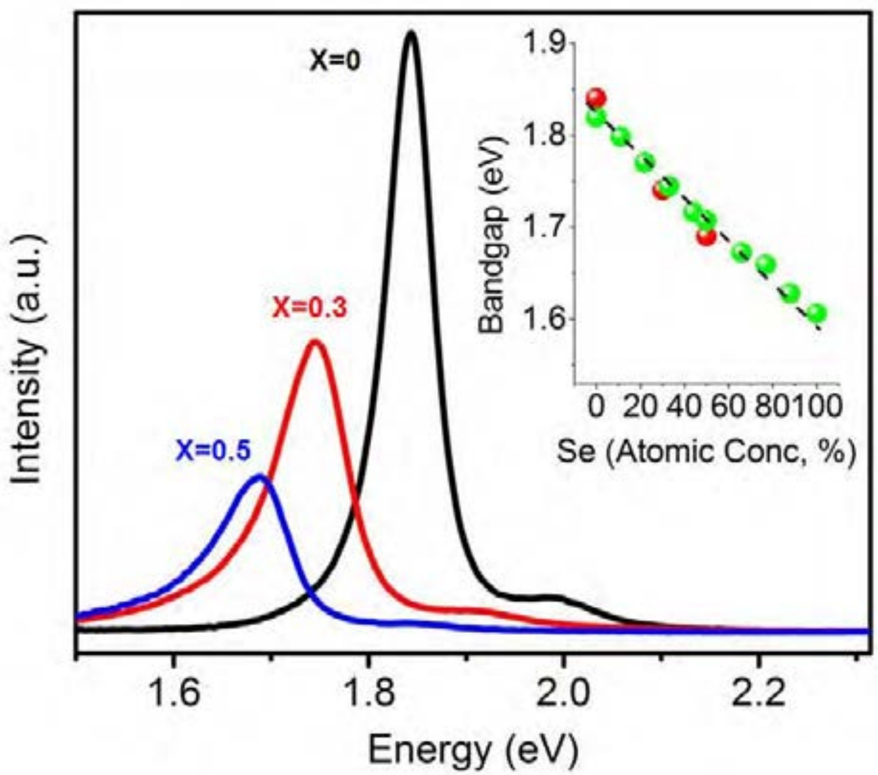


red: Mo
dark green: S+S
bright green :S+Se
white: Se+Se

Yongji Gong†, Zheng Liu, Wu Zhou, Gang Shi, Sina Najmaei, Zhong Lin, Ana Laura Elías, Ayse Berkdemir, Ge You, Humberto Terrones, Mauricio Terrones, Robert Vajtai, Jun Lou, Pulickel M. Ajayan.
Nano Letters (2014)

PL of $MoS_{2(1-x)}Se_x$ atomic layers

Terrones & Ajayan



- **Challenges remaining**

Can we control the positions of Se and S?

Can we have a segregated monolayer of Se and S on top and bottom?

What are the driving forces to promote Se and S segregation?

Yongji Gong†, Zheng Liu, Wu Zhou, Gang Shi, Sina Najmaei, Zhong Lin, Ana Laura Elías, Ayse Berkdemir, Ge You, Humberto Terrones, Mauricio Terrones, Robert Vajtai, Jun Lou, Pulickel M. Ajayan.
Nano Letters (2014)

Mn-doped MoS_2

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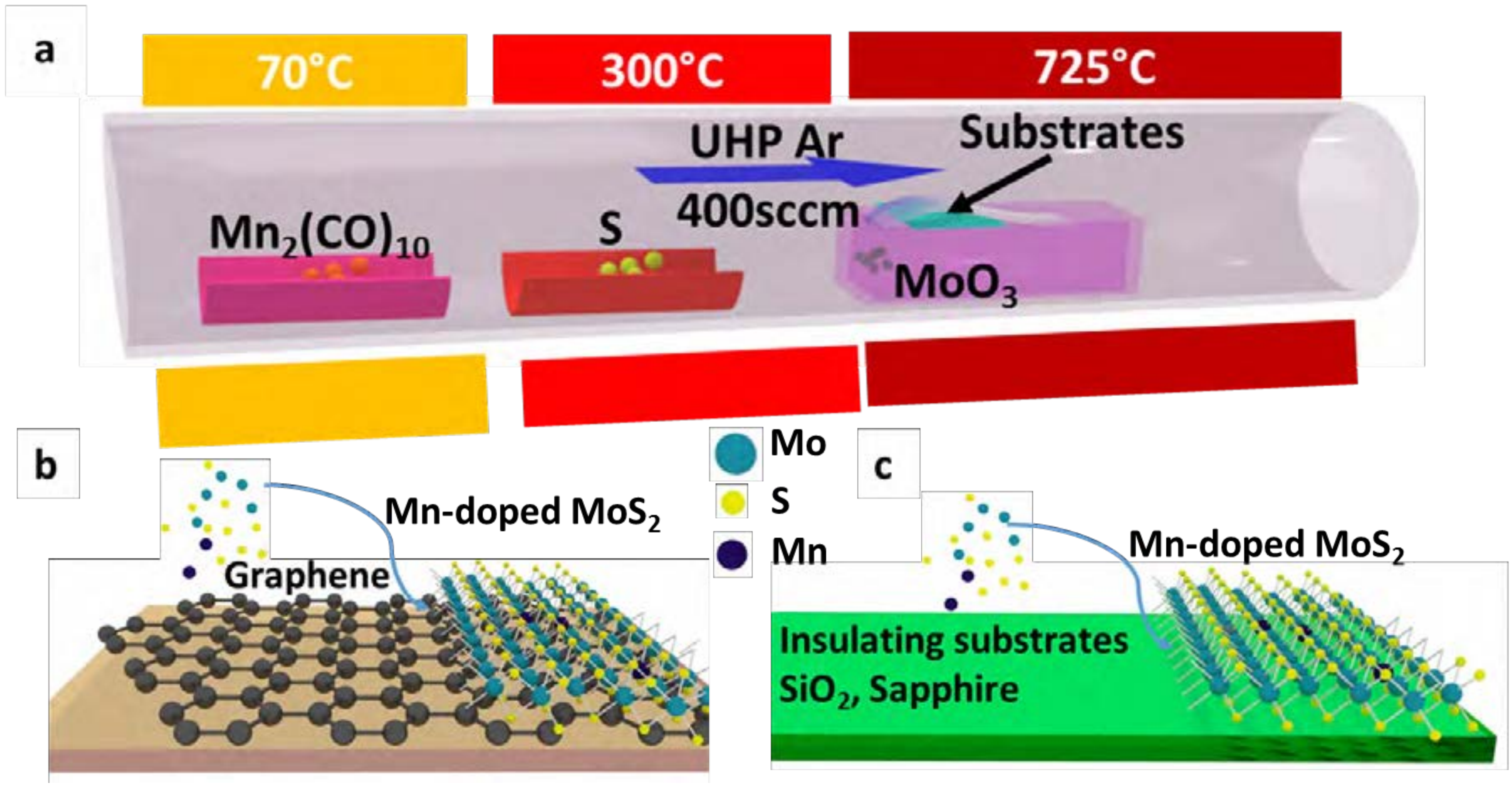
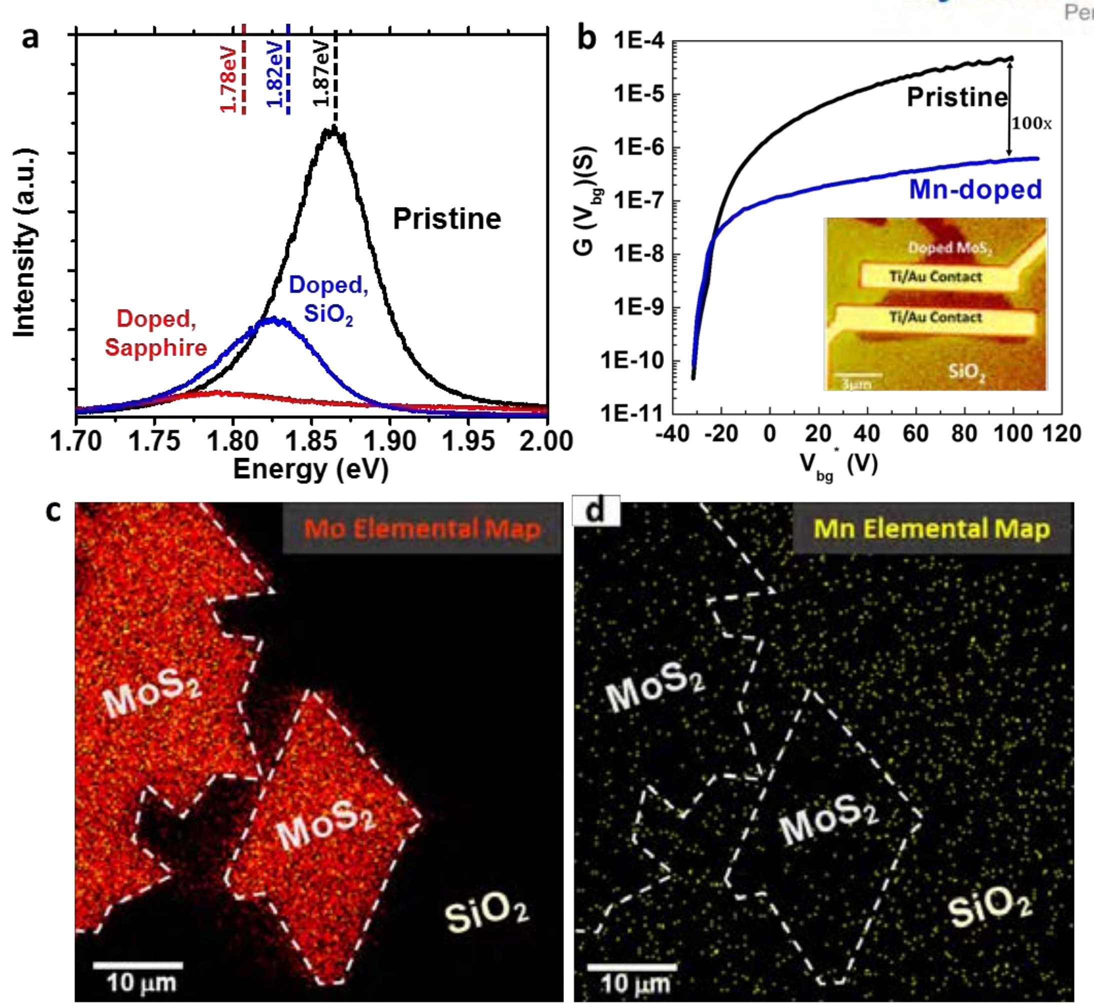


- The presence of Mn promotes the growth of monolayered triangular MoS_2 and WS_2 islands.

K.Zhang, S. Feng, M. Terrones, J. Zhu, J.A. Robinson, et al., Nano Lett (2015)

Mn-doped MoS_2 : PL & Transport changes



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Mn-doped MoS_2 : PL & Transport changes

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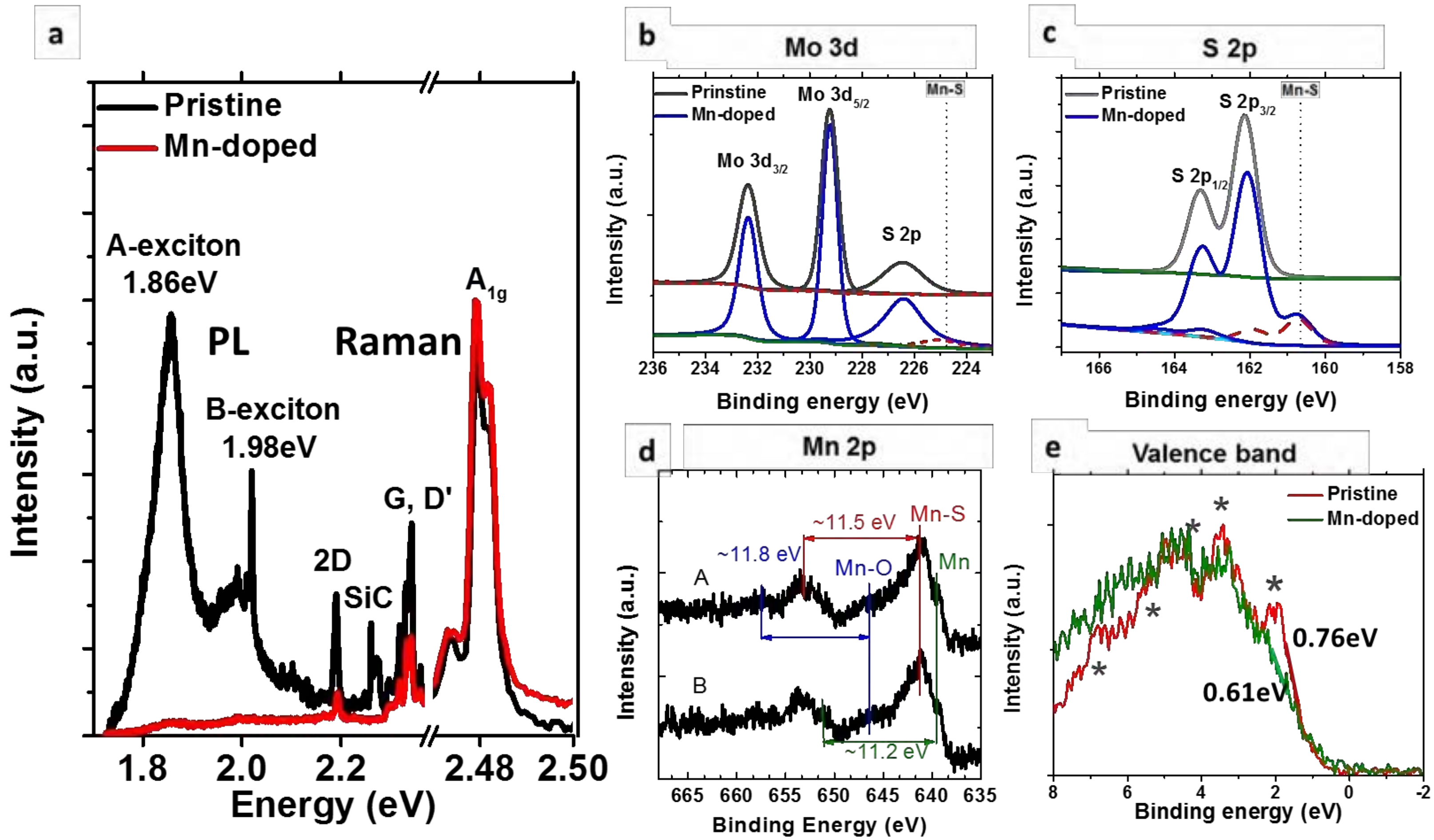

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K.Zhang, S. Feng, M. Terrones, J. Zhu, J.A. Robinson, et al., Nano Lett (2015)

Mn-doped MoS_2 : Grain Boundaries

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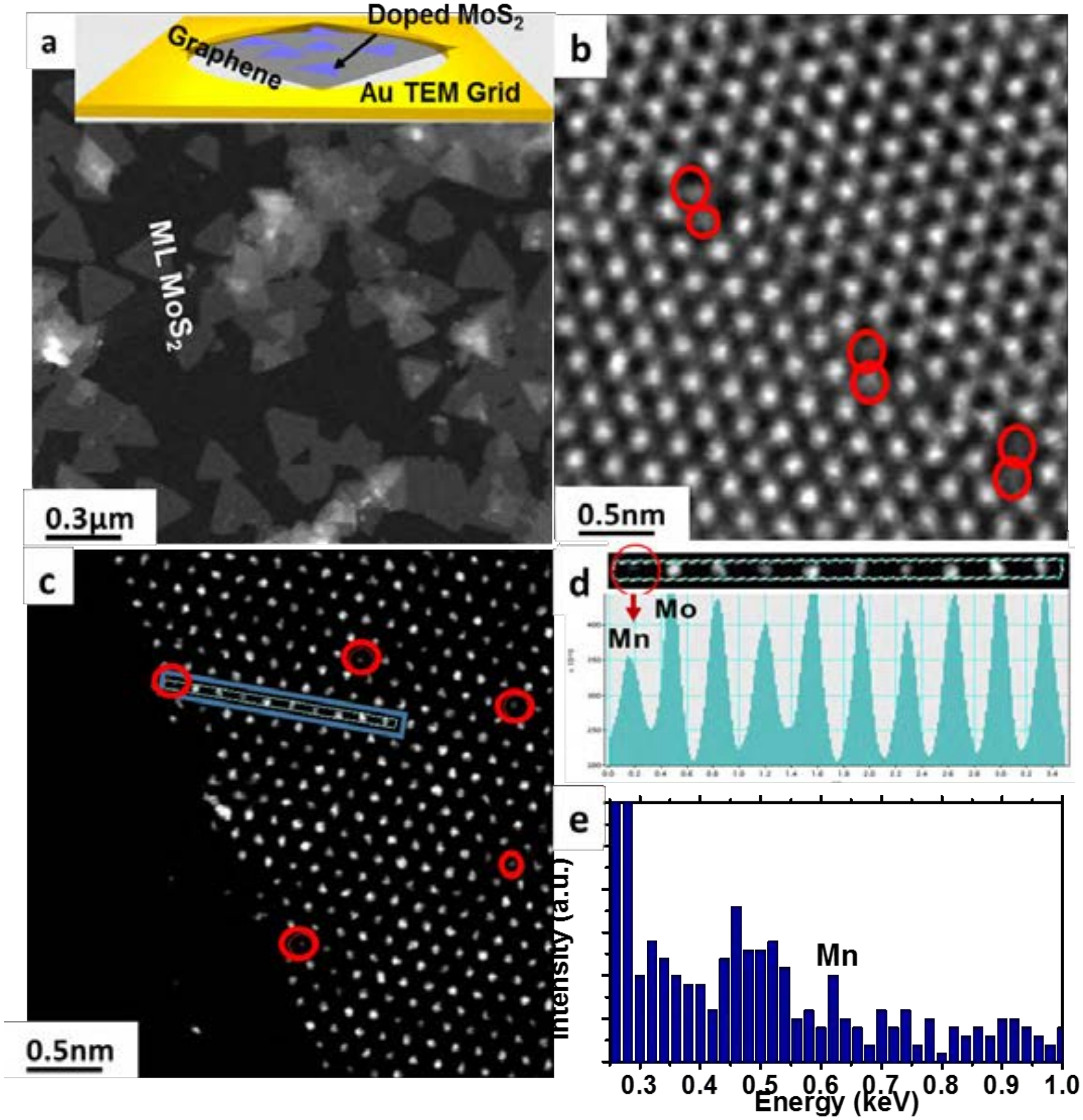


- **Challenges remaining**

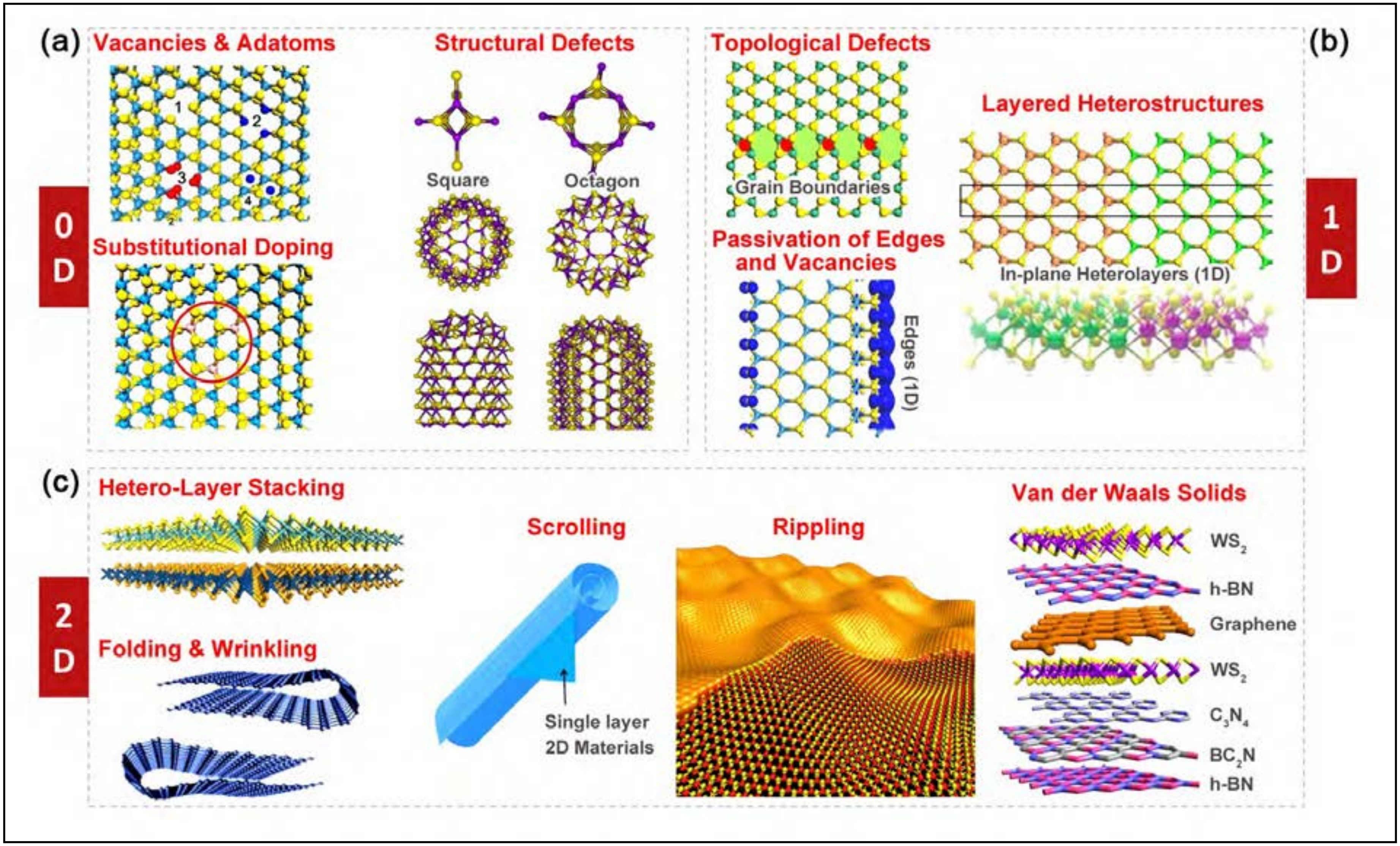
Can we add more Mn in the structure?

What would the magnetic properties be when Mn is around 10% at.?

➢ **Mn is embedded in the lattice**

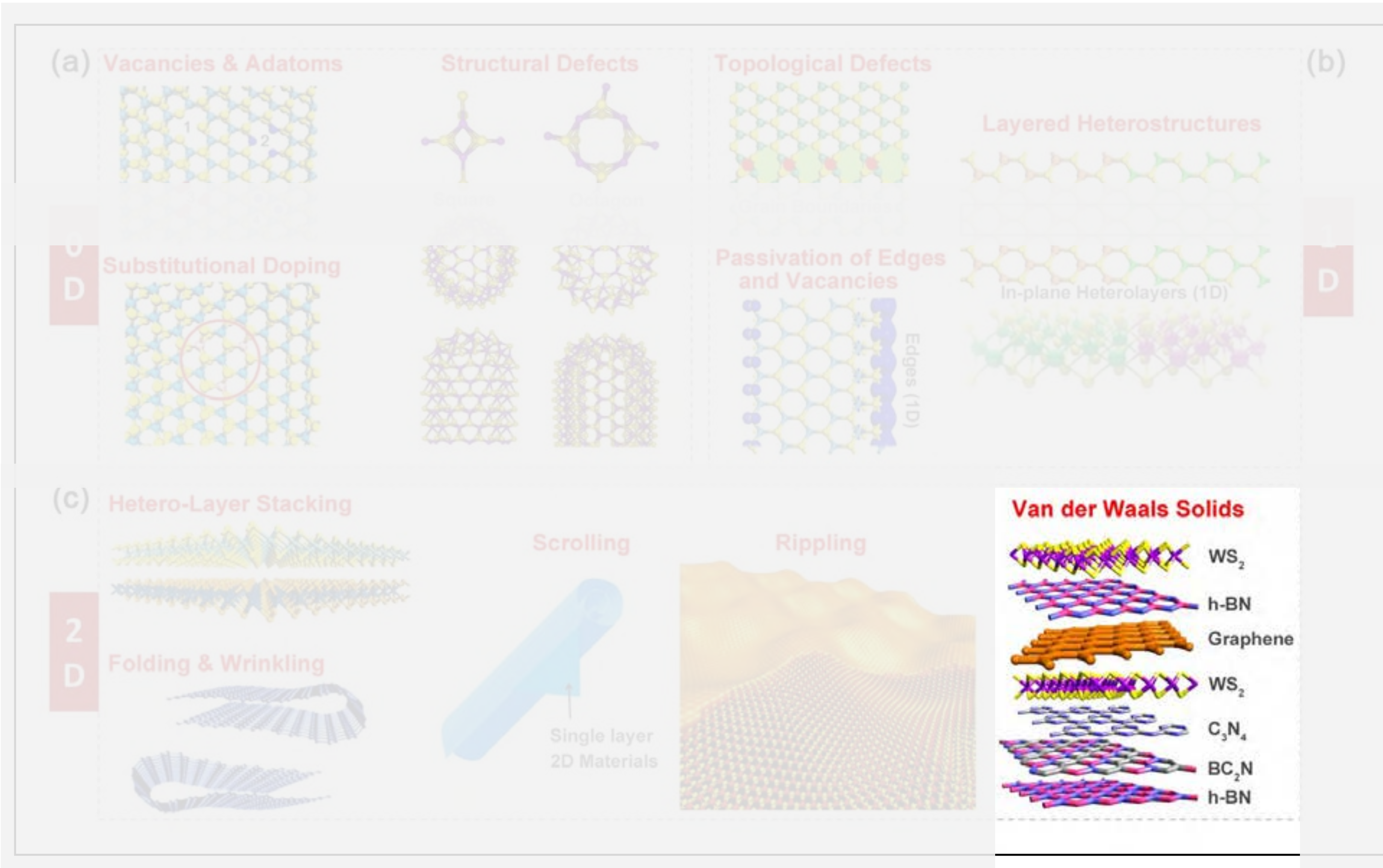
K.Zhang, S. Feng, M. Terrones, J. Zhu, J.A. Robinson, et al., Nano Lett (2015)

Defect Engineering



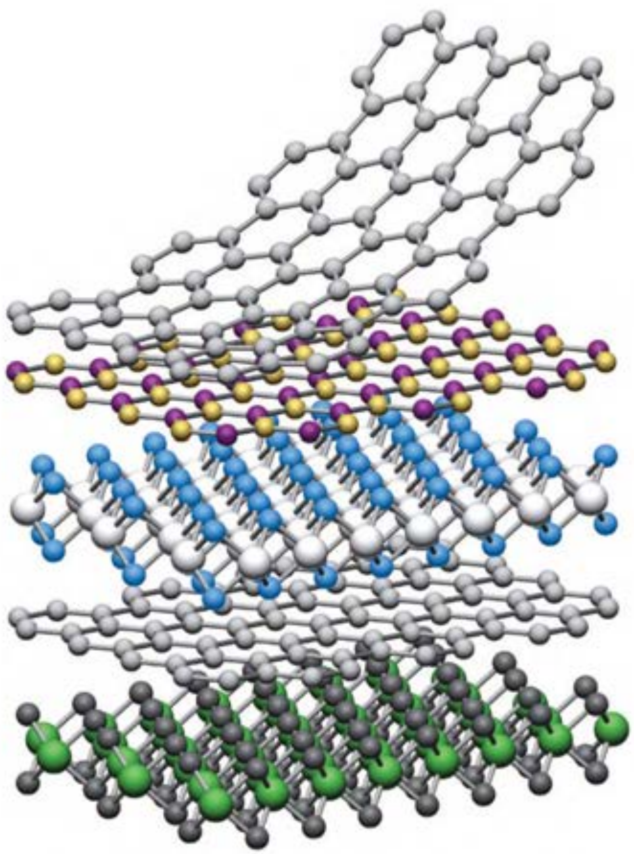
Z. Lin, B.R. Carvalho, E. Kahn, R. Lv, R. Rao, H. Terrones, M.A. Pimenta, M. Terrones. 2D Materials (2016)

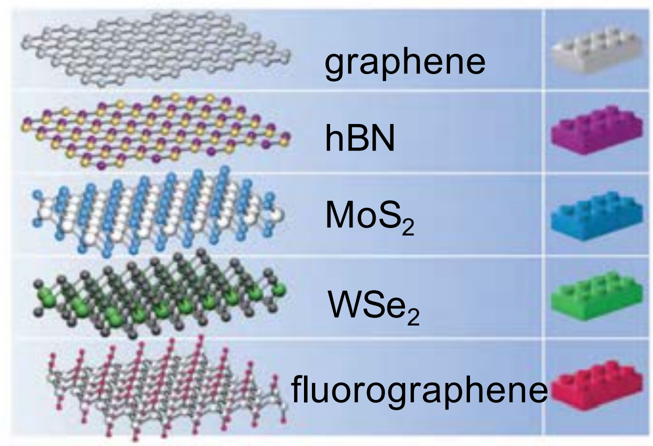
Defect Engineering

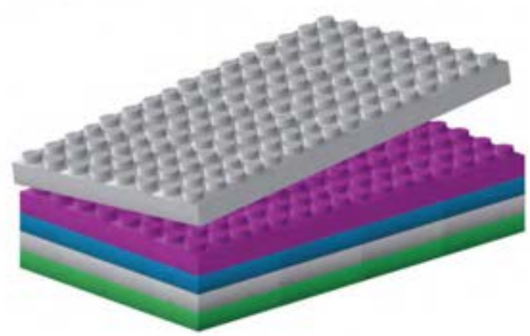


Z. Lin, B.R. Carvalho, E. Kahn, R. Lv, R. Rao, H. Terrones, M.A. Pimenta, M. Terrones. 2D Materials (2016)

Van der Waals Heterostructures

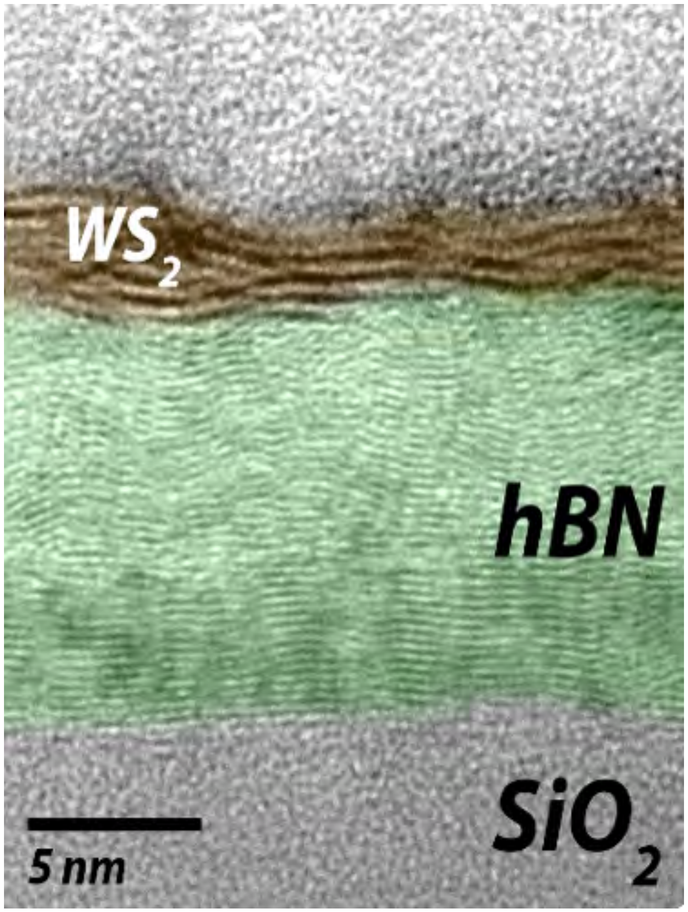


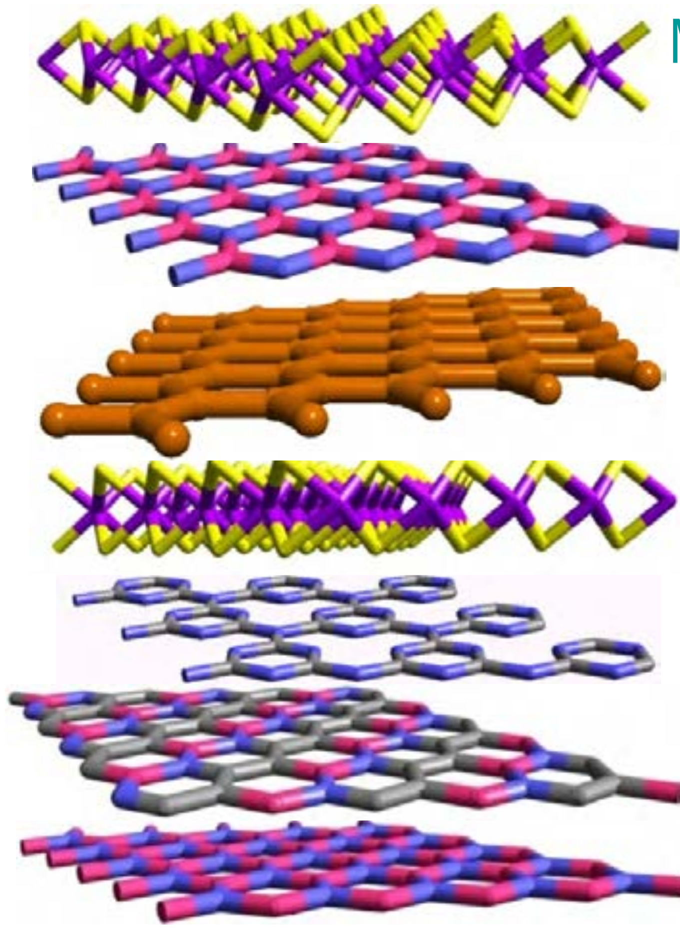




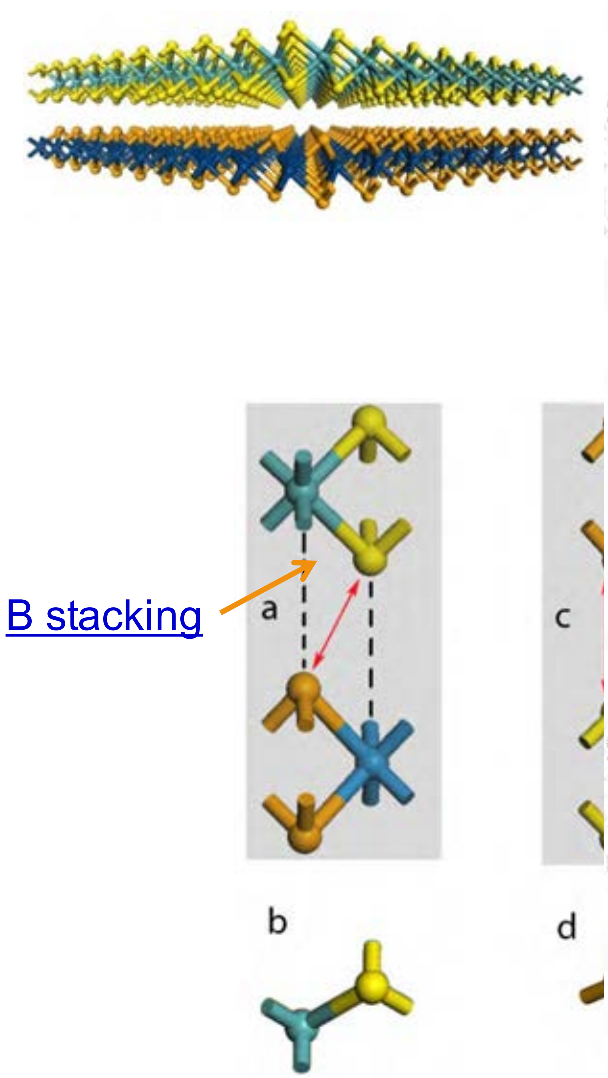
Geim, et al. Nature, 499 (2013) 419.
http://www.papermachine.com.cn

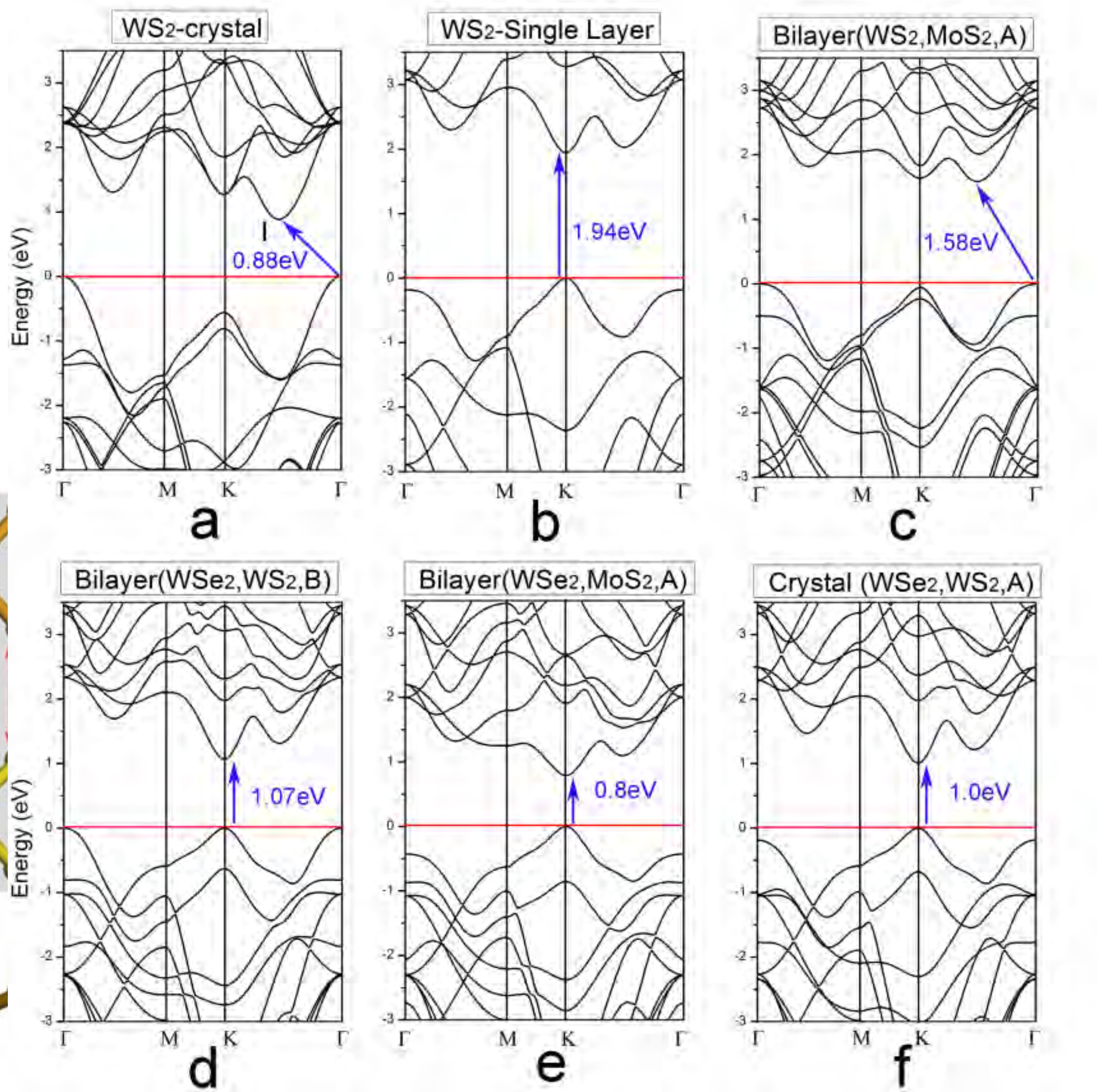
Synthesis of Hybrid and Doped 2D Systems





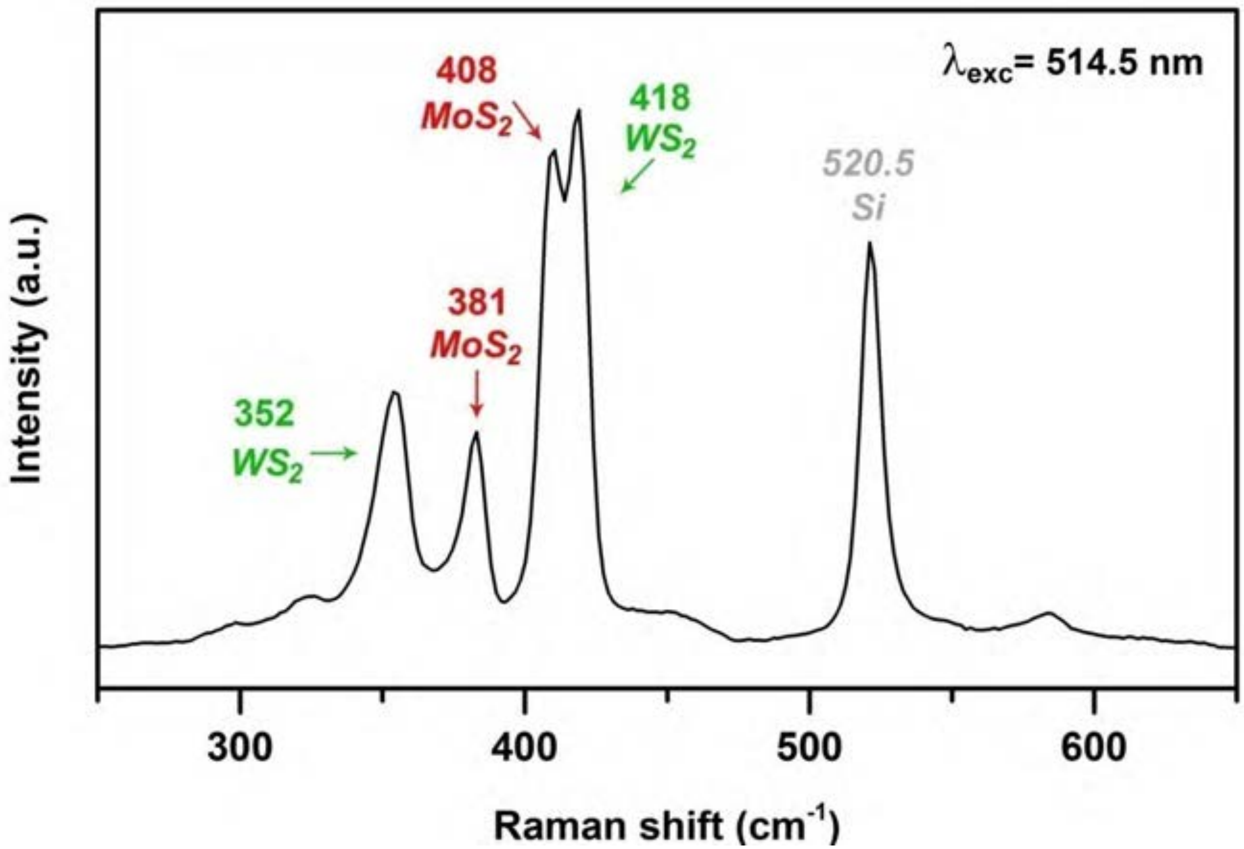
New Materials: Heterostructures of TMD

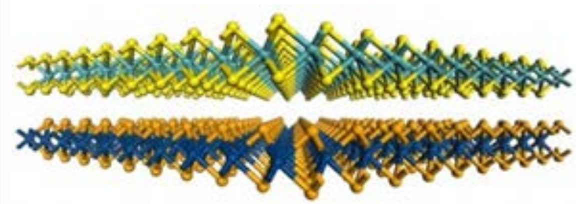




H. Terrones, F. Lopez-Urias, M.Terrones. Nature Scientific Reports 3, 1549 (2013).

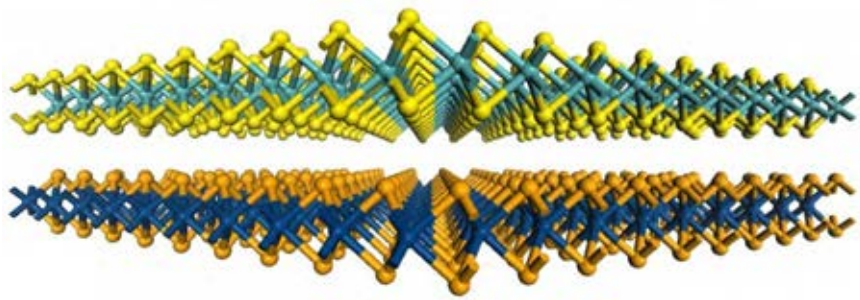
Controlled growth of Hybrid Layers of Mo-W-S_2 by low pressure CVD: Raman Spectroscopy

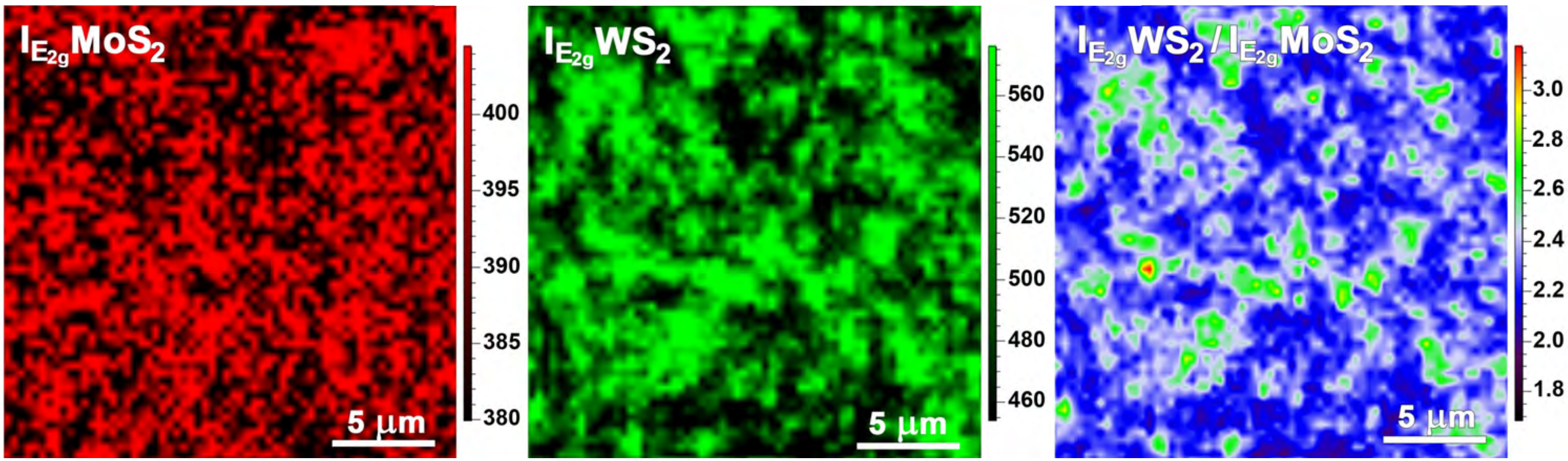




A.L. Elías, N. Perea-López, A. Castro-Beltrán, A. Berkdemir, R. Lv, S. Feng, A. Long, T. Hayashi, Y. A. Kim, M. Endo, H. R. Gutiérrez, N. R. Pradhan, L. Balicas, T. E. Mallouk, F. López-Urías, H. Terrones, M.Terrones. ACS Nano ASAP (2013)

Controlled growth of Hybrid Layers of Mo-W-S_2 by low pressure CVD: Raman Spectroscopy Mapping





A.L. Elías, N. Perea-López, A. Castro-Beltrán, A. Berkdemir, R. Lv, S. Feng, A. Long, T. Hayashi, Y. A. Kim, M. Endo, H. R. Gutiérrez, N. R. Pradhan, L. Balicas, T. E. Mallouk, F. López-Urías, H. Terrones, M.Terrones. ACS Nano ASAP (2013)

MoS_2/Epi-Graphene

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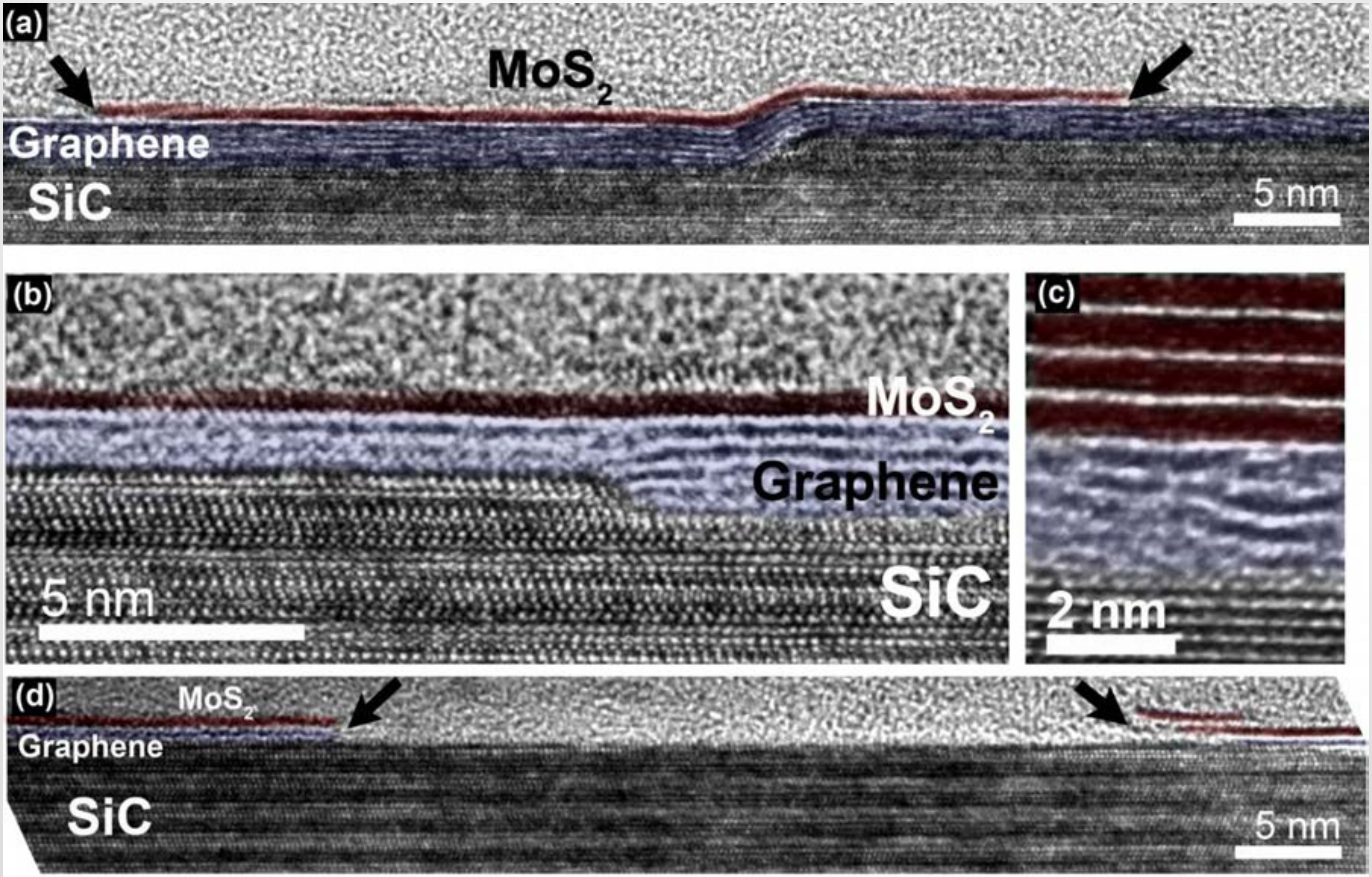
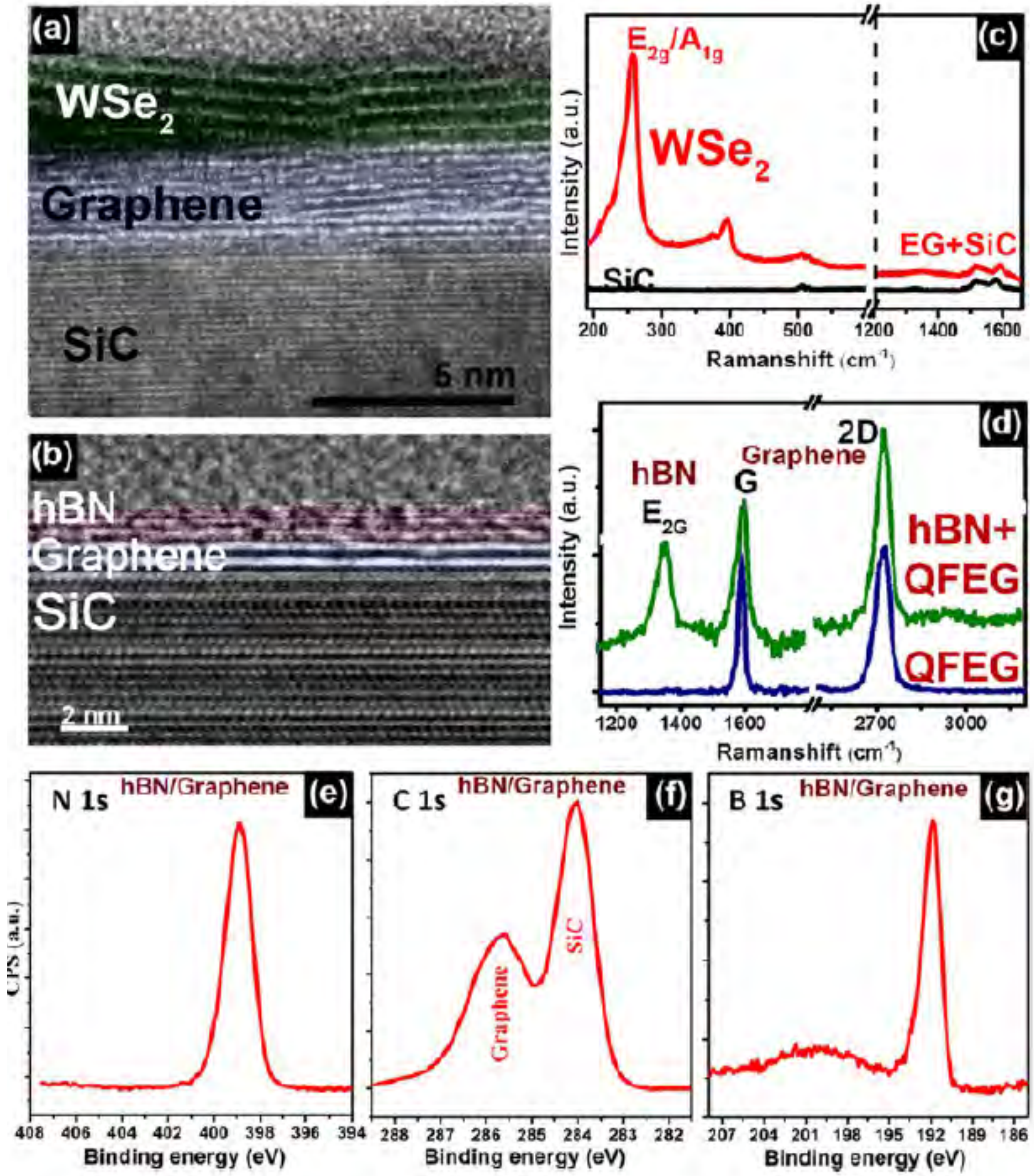


Collaboration with J.A. Robinson

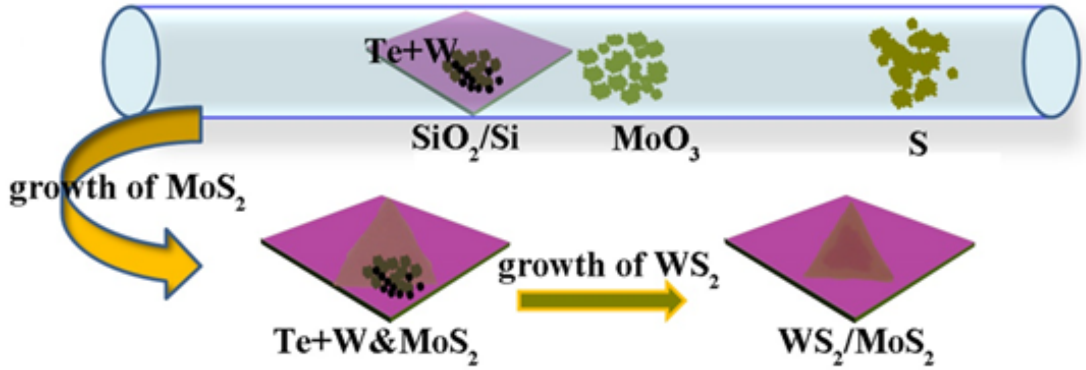
Direct Growth of vdW Solids on Expitaxial Graphene

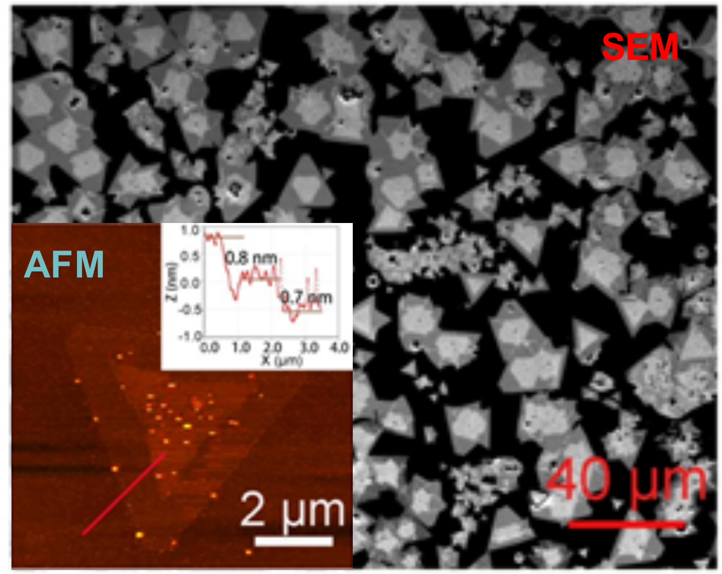


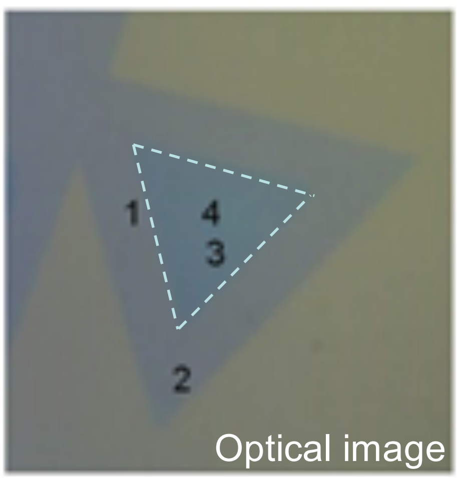
Collaboration with J.A. Robinson

Lin, et al. Acs Nano. (2014)

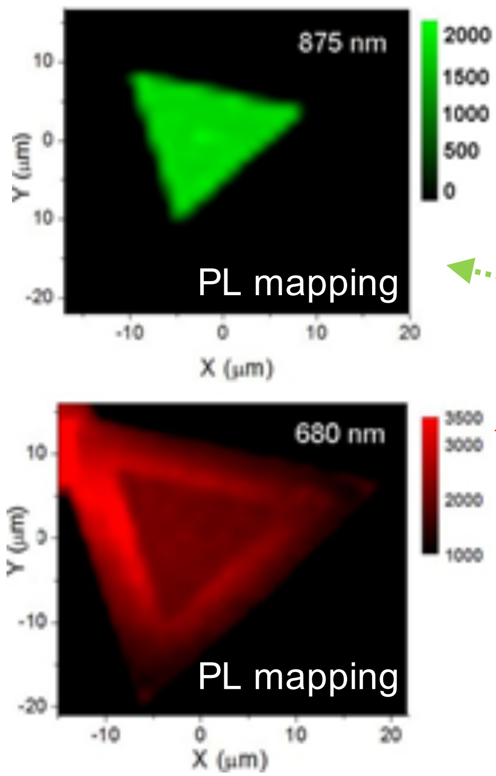
Large Scale Synthesis of MoS_2/WS_2 Vertical Heterostructures

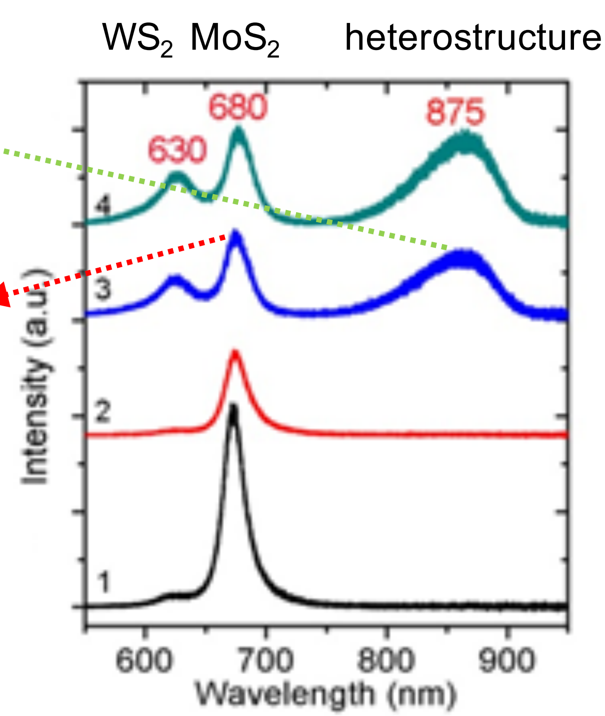


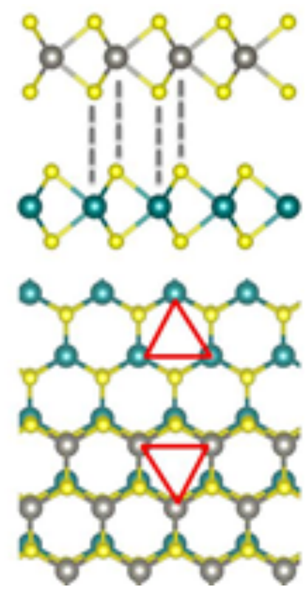




1&2 monolayer MoS_2
3&4 MoS_2/WS_2



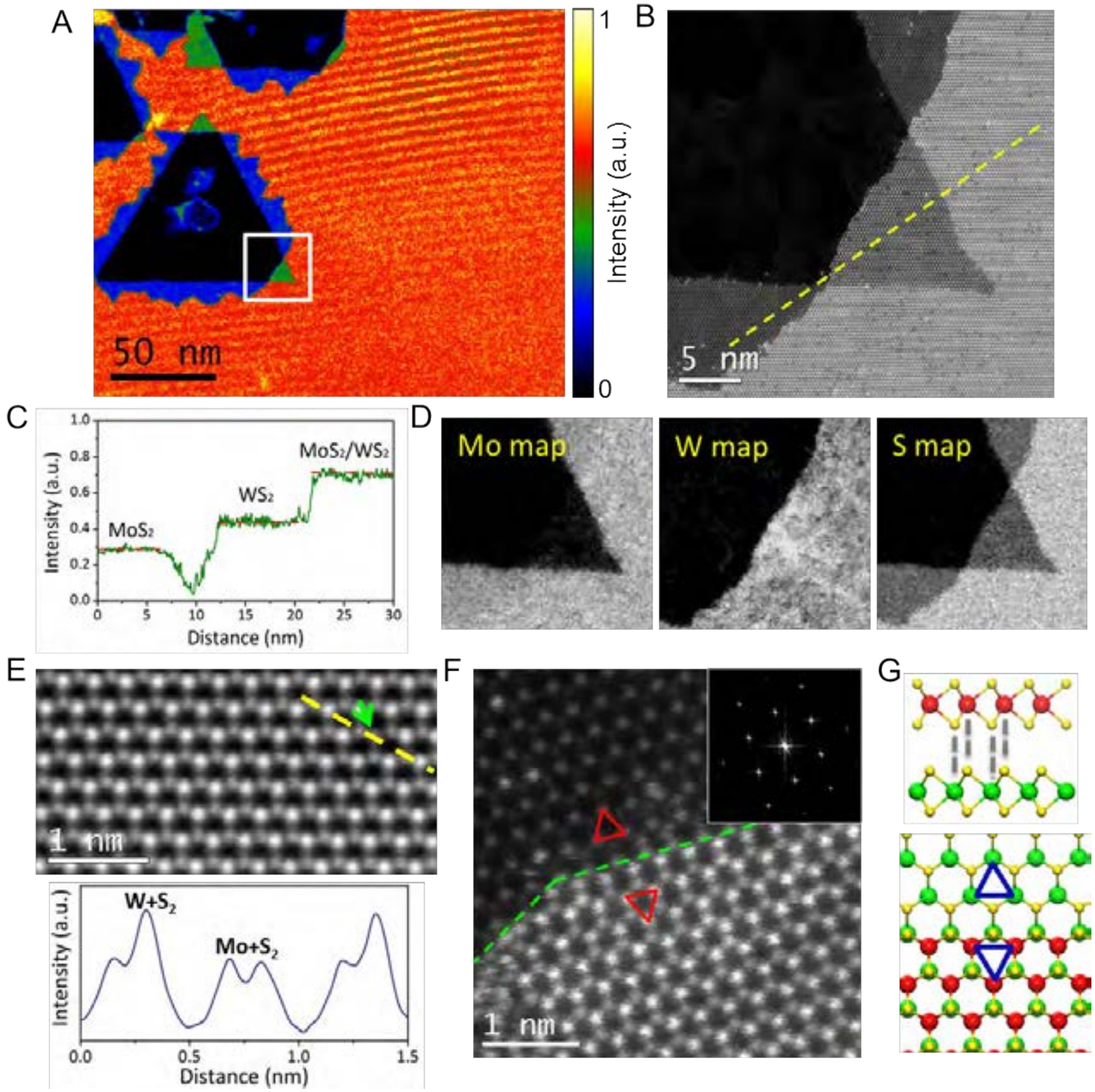




2H stacking

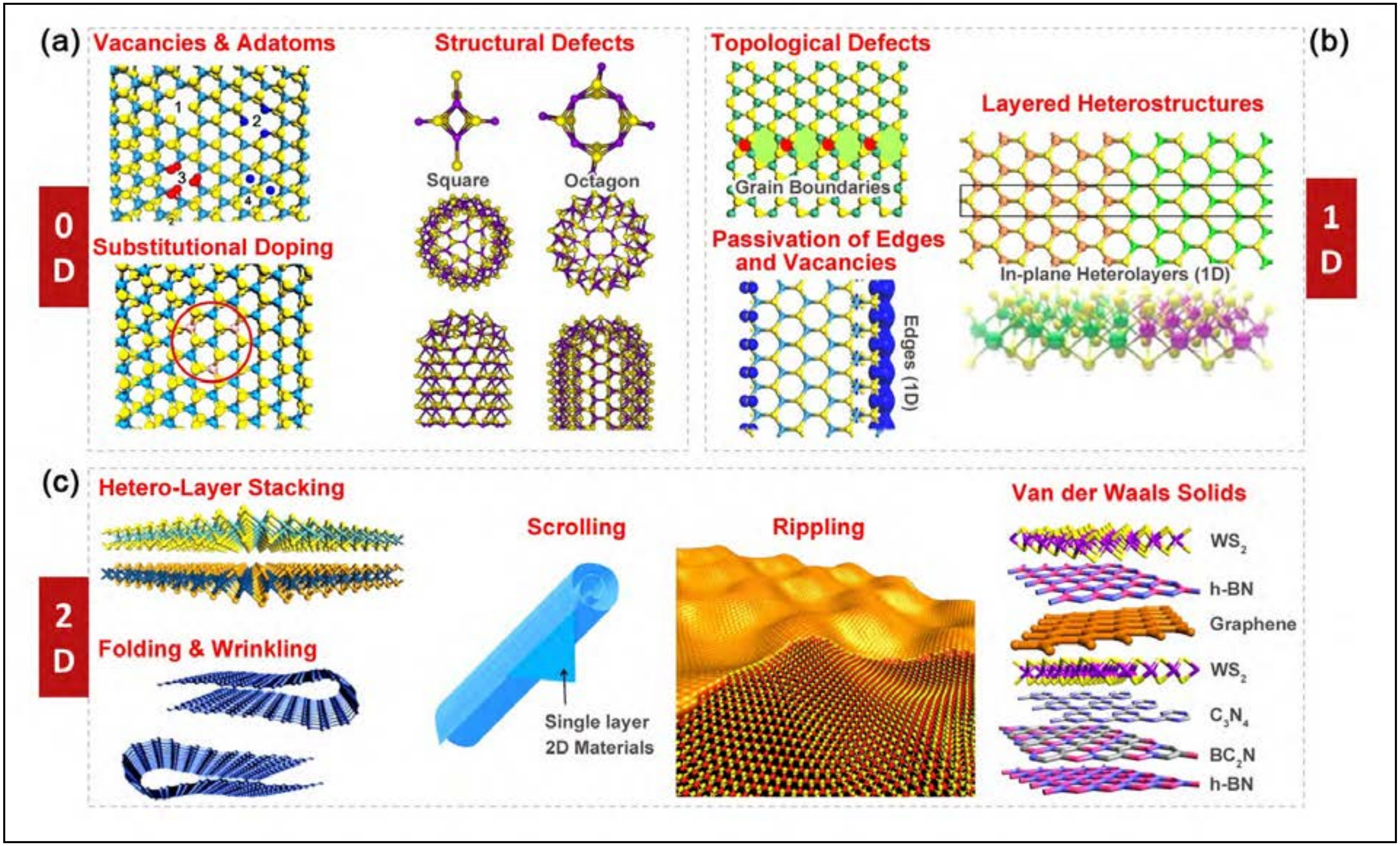
Gong, et al. Nature Materials (2014)

Large Scale Synthesis of MoS_2/WS_2 Vertical Heterostructures



Gong, et al. Nature Materials (2014)

Defect Engineering



Z. Lin, B.R. Carvalho, E. Kahn, R. Lv, R. Rao, H. Terrones, M.A. Pimenta, M. Terrones. 2D Materials (2016)

Possible Defect Structure in TMDs

Center for 2-Dimensional and Layered Materials Penn State

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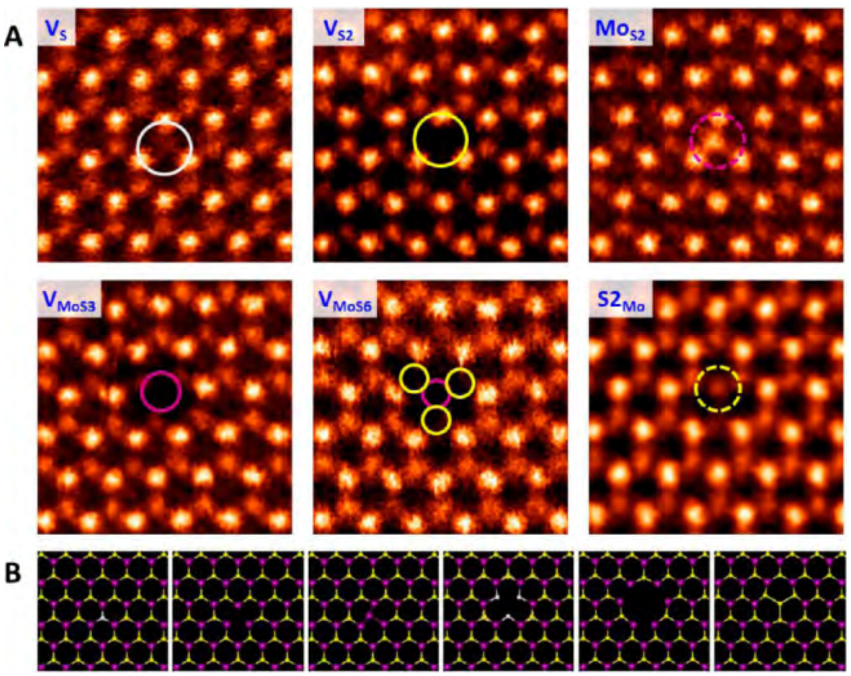
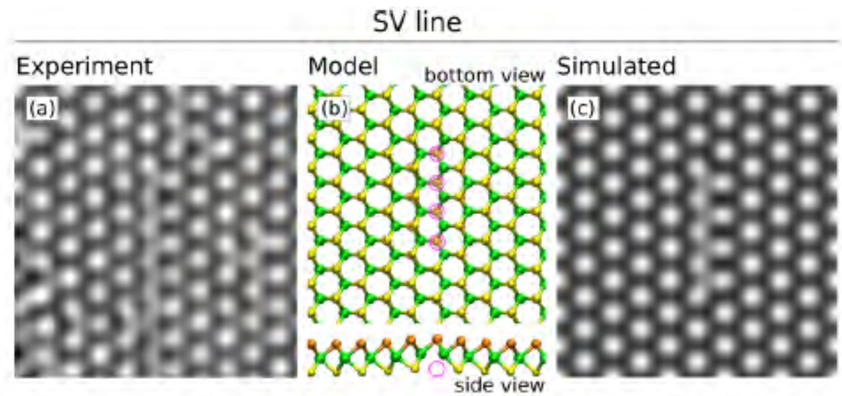
- **Atomic defect (vacancy, substitution)**



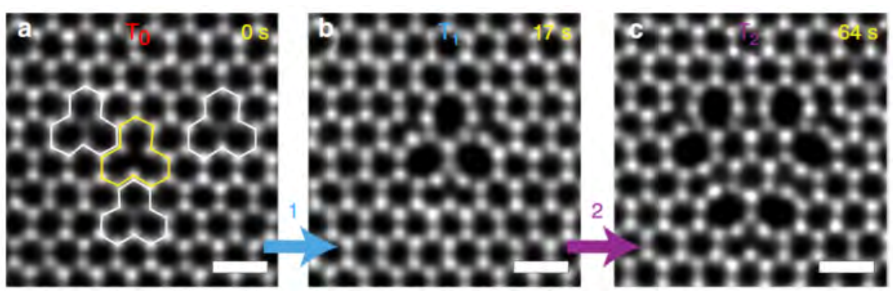
W.Zhou, et al., Nano Lett. (2013)

- **Lined vacancies**



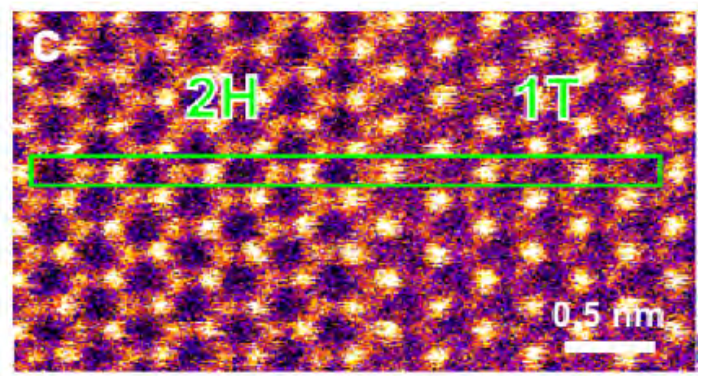
H-P. Komsa, et al., Phys.Rev.B (2013)

- **Aggregated vacancies**



Y.-C.Lin, et al., *Nat.Commn.* (2015)

- **Phase transition**



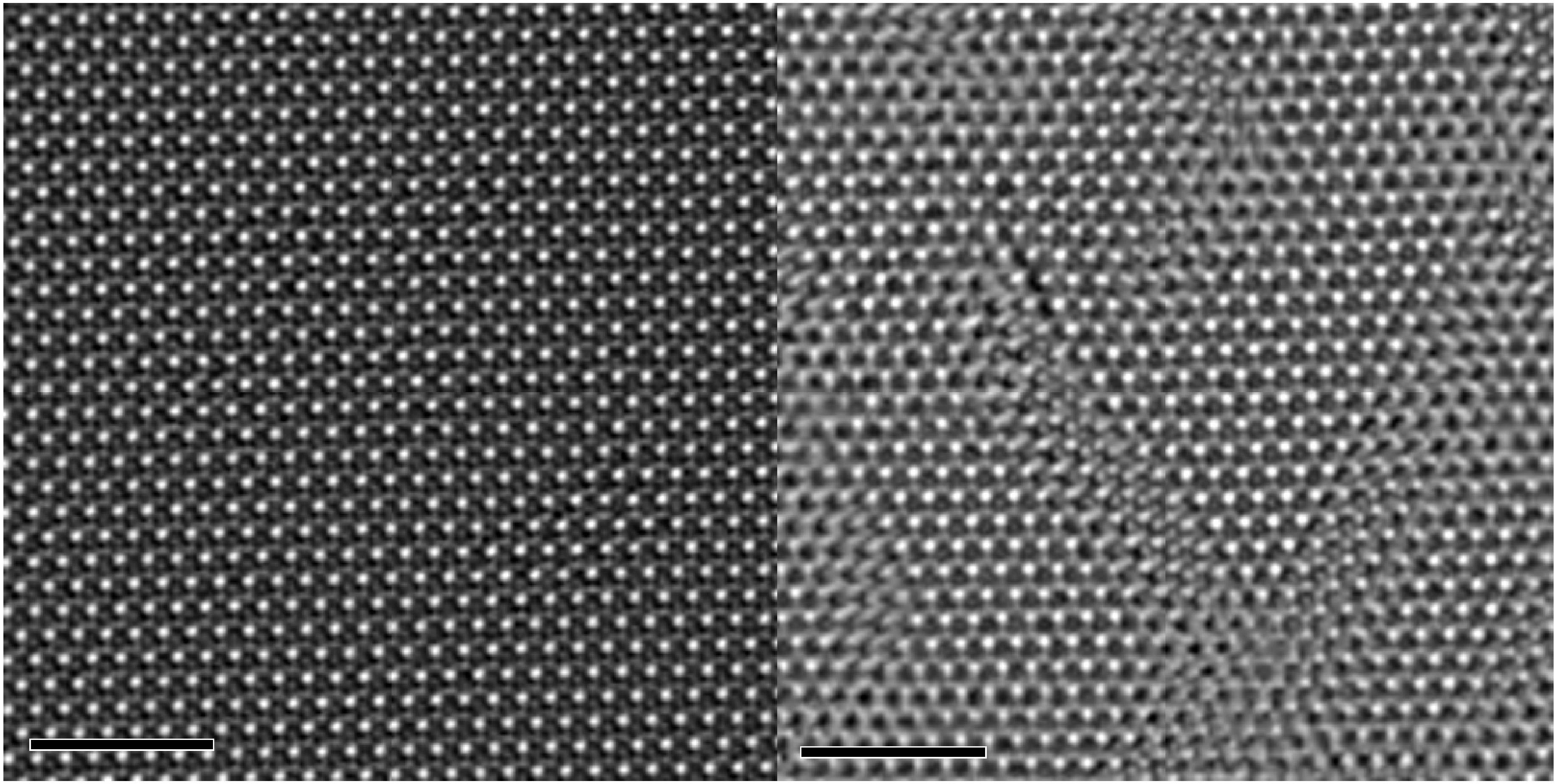
Y.-C.Lin, et al., *Nat.Nanotech.* (2014)

K.Fujisawa, B.Kabius, V.Carozo, S.Feng, Z.Lin, C.Zhou, M.Terrones, et al., unpublished (2015)

Structural Change after E-beam Irradiation

No damage area

E-beam damaged area



- WS_2 structure was changed by E-beam irradiation. Details should be studied with TEM simulation.

K.Fujisawa, B.Kabius, V.Carozo, S.Feng, Z.Lin, C.Zhou, M.Terrones, et al., unpublished (2015)

Atomic-vacancy Healing in MoS_2

Center for 2-Dimensional and Layered Materials Penn State

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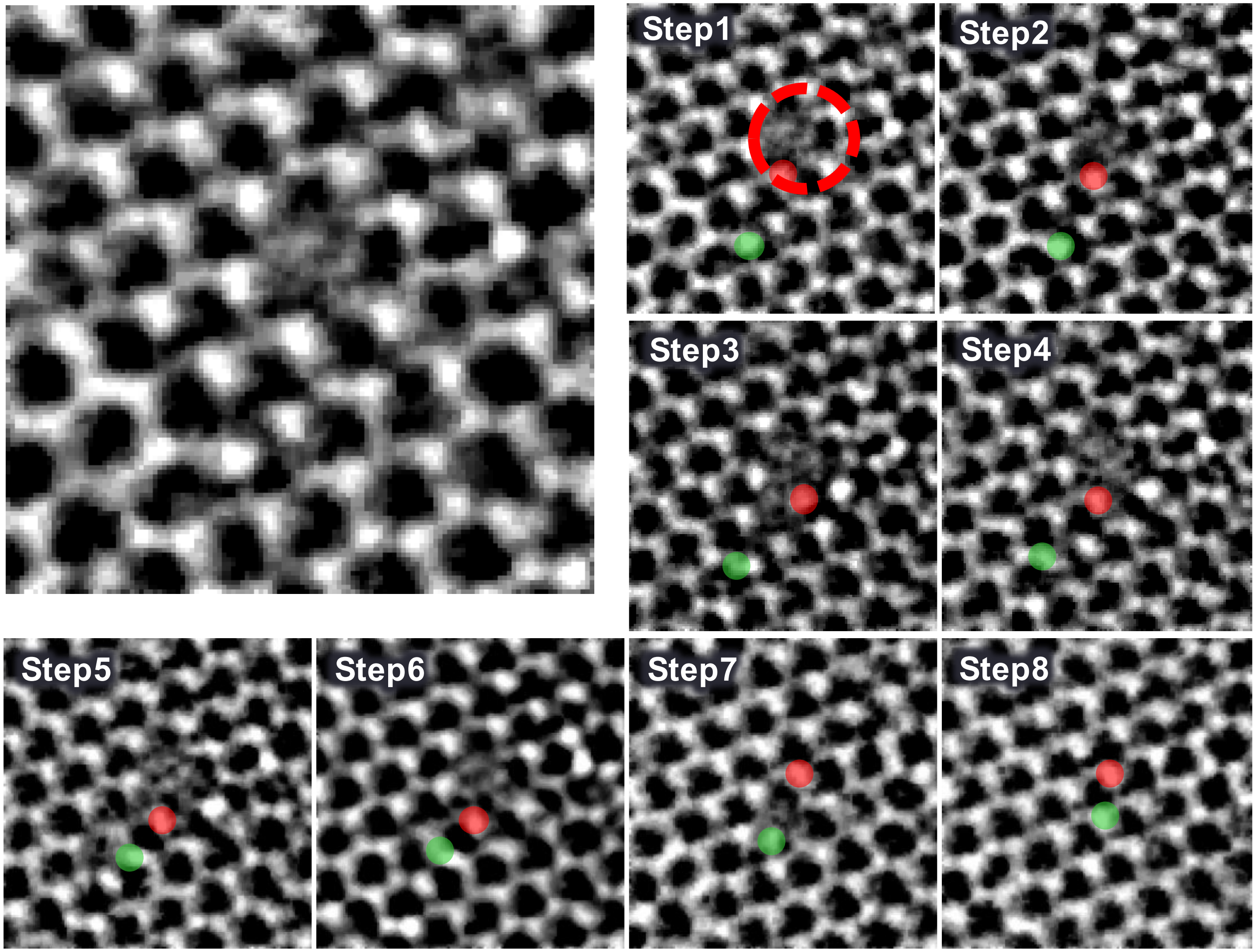


- Mo atom

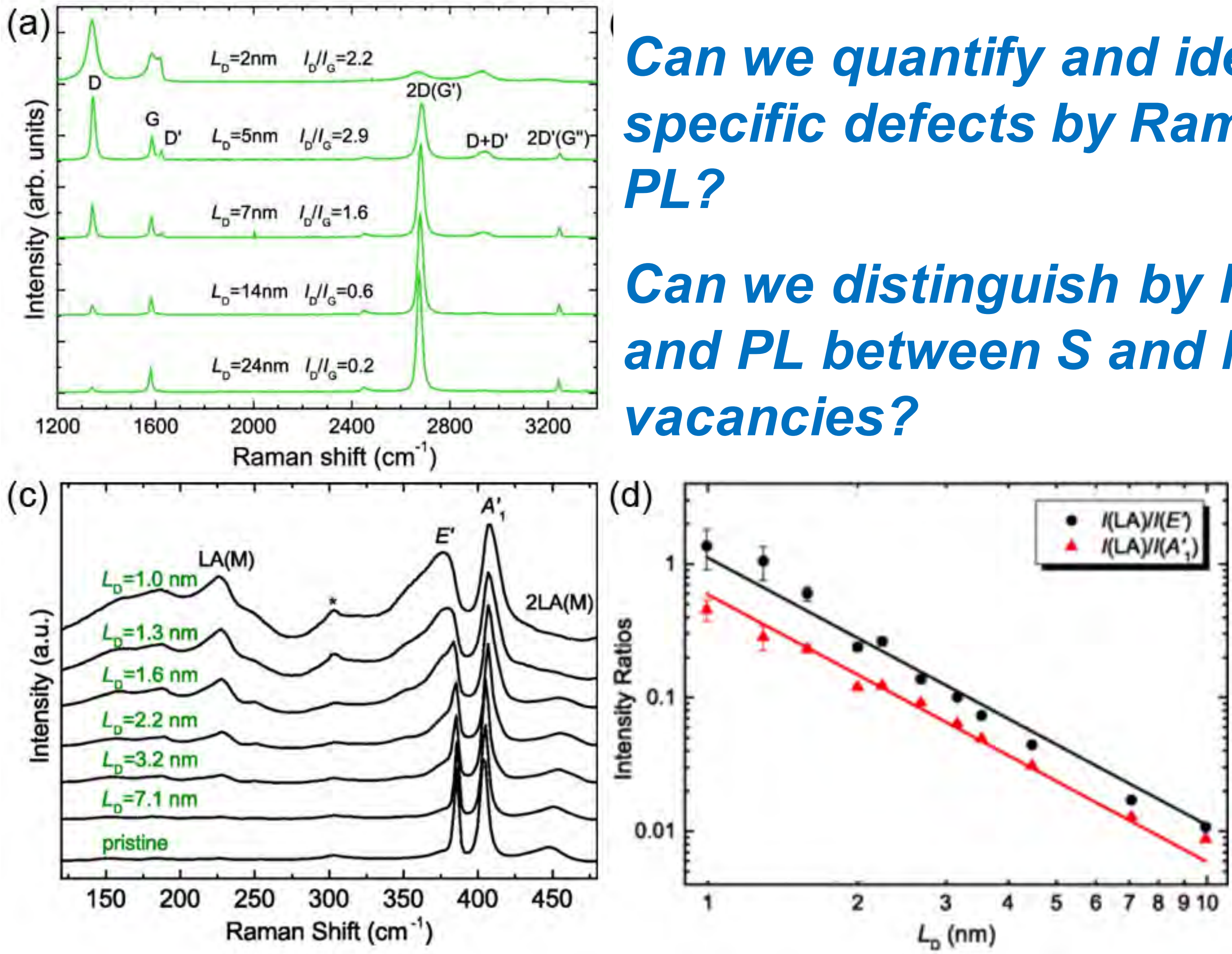
K.Fujisawa, B.Kabius, V.Carozo, S.Feng, Z.Lin, C.Zhou, M.Terrones, et al., unpublished (2015)

Defects on TMDs, MoS_2-type

- **Challenges remaining**

Can we quantify and identify specific defects by Raman and PL?

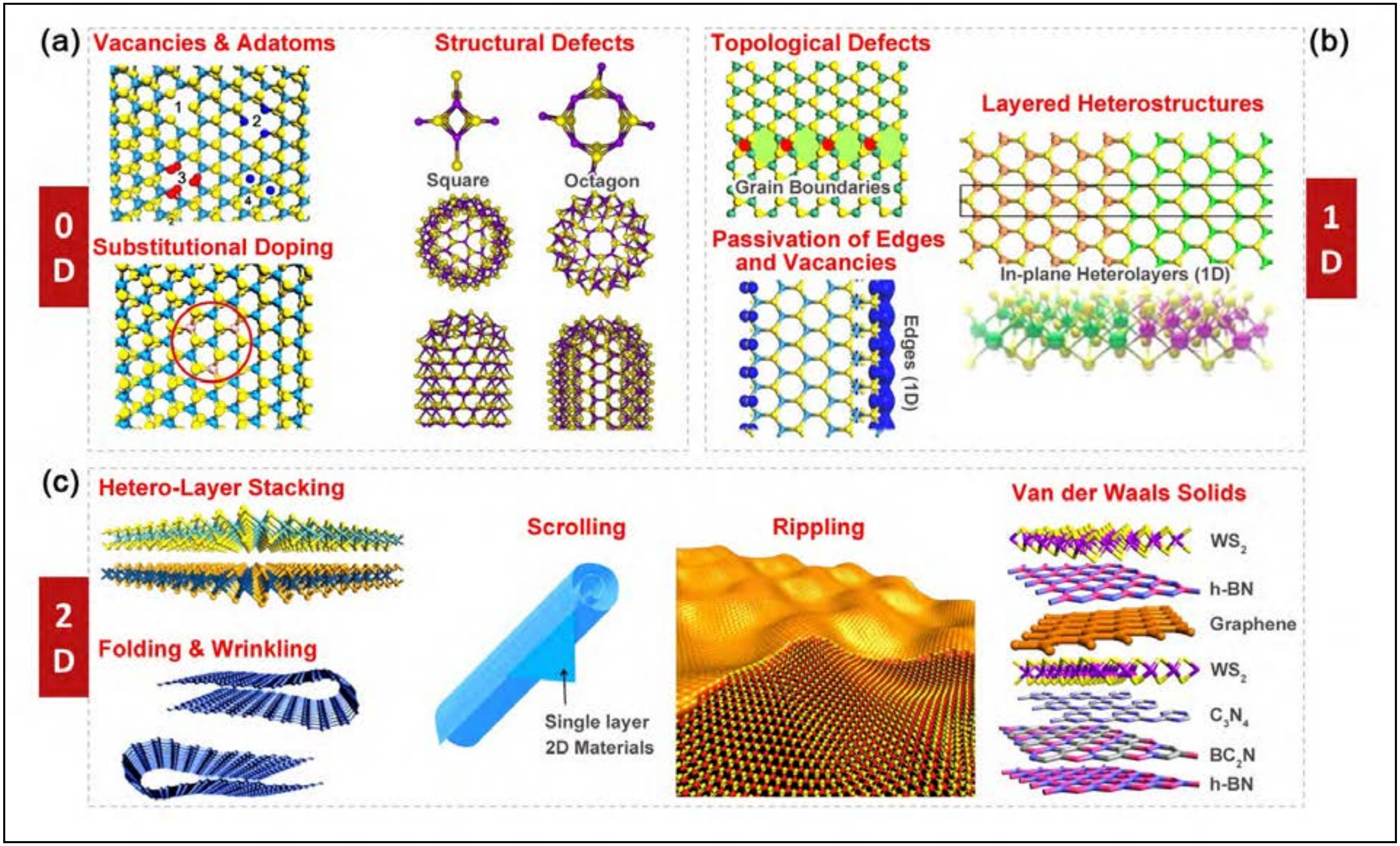
Can we distinguish by Raman and PL between S and M vacancies?



The LA mode appears after the ion-bombardment

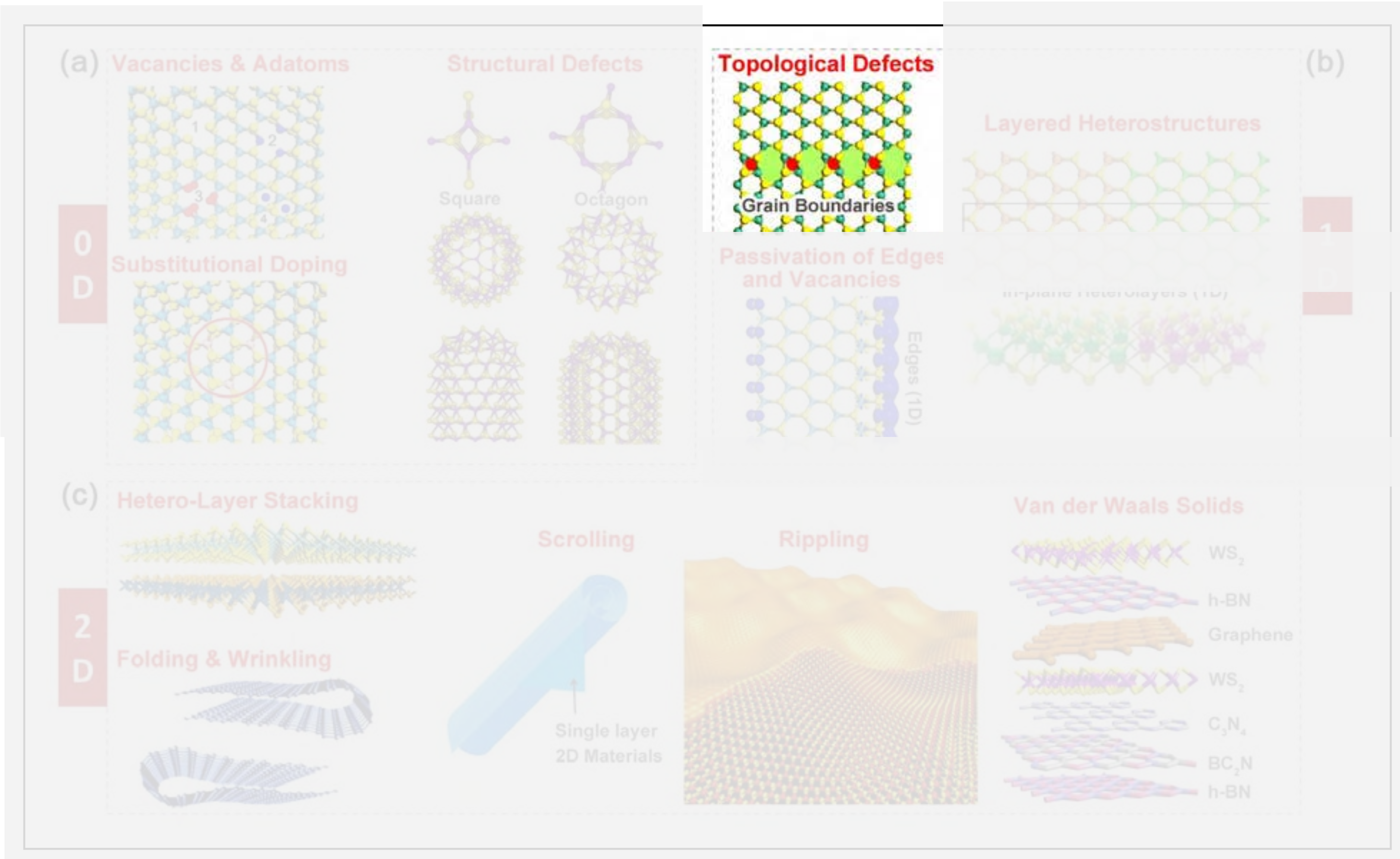
B. Carvalho, N. Perea-López, Z. Lin, K. Fujisawa, V. Carozo, A. Elías, and M. Terrones et al., unpublished (2015)

Defect Engineering



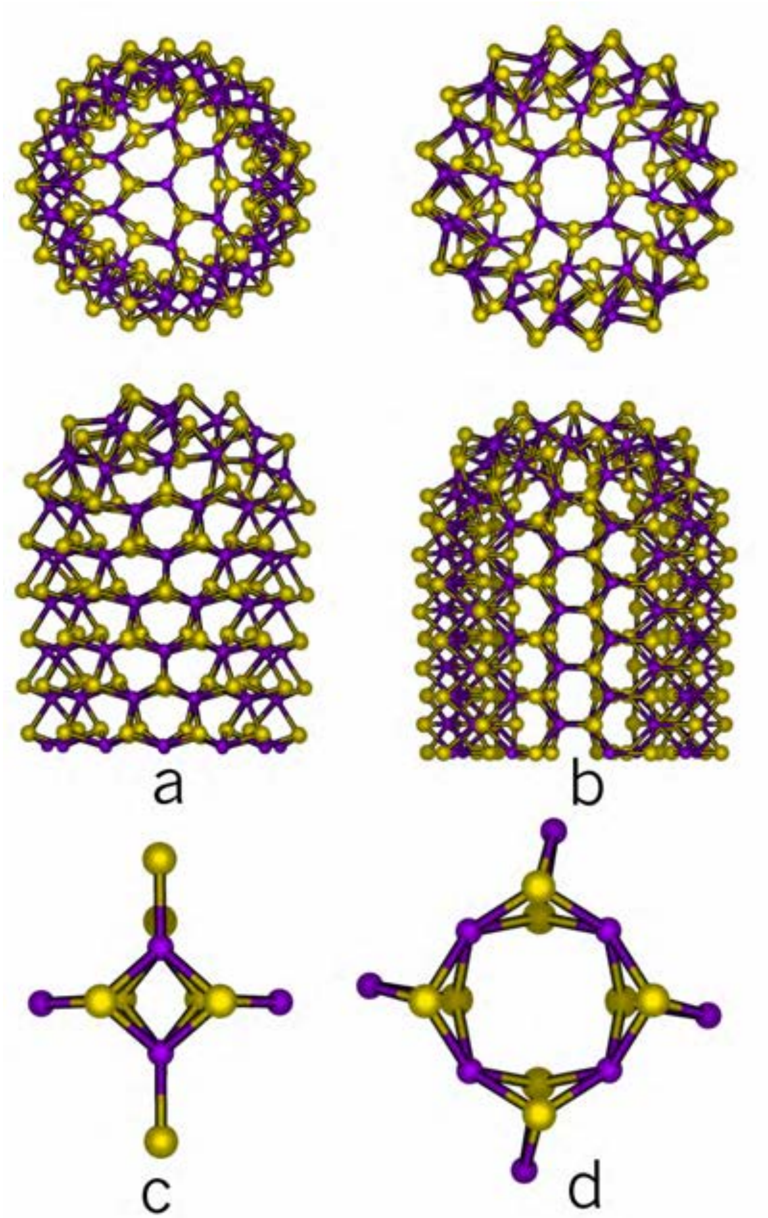
Z. Lin, B.R. Carvalho, E. Kahn, R. Lv, R. Rao, H. Terrones, M.A. Pimenta, M. Terrones. 2D Materials (2016)

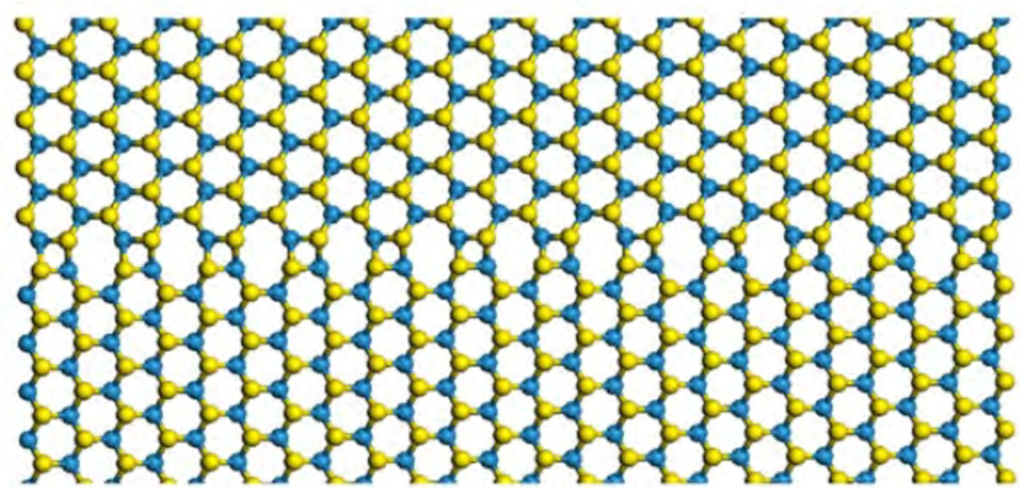
Defect Engineering



Z. Lin, B.R. Carvalho, E. Kahn, R. Lv, R. Rao, H. Terrones, M.A. Pimenta, M. Terrones. 2D Materials (2016)

Topological defects in TMD

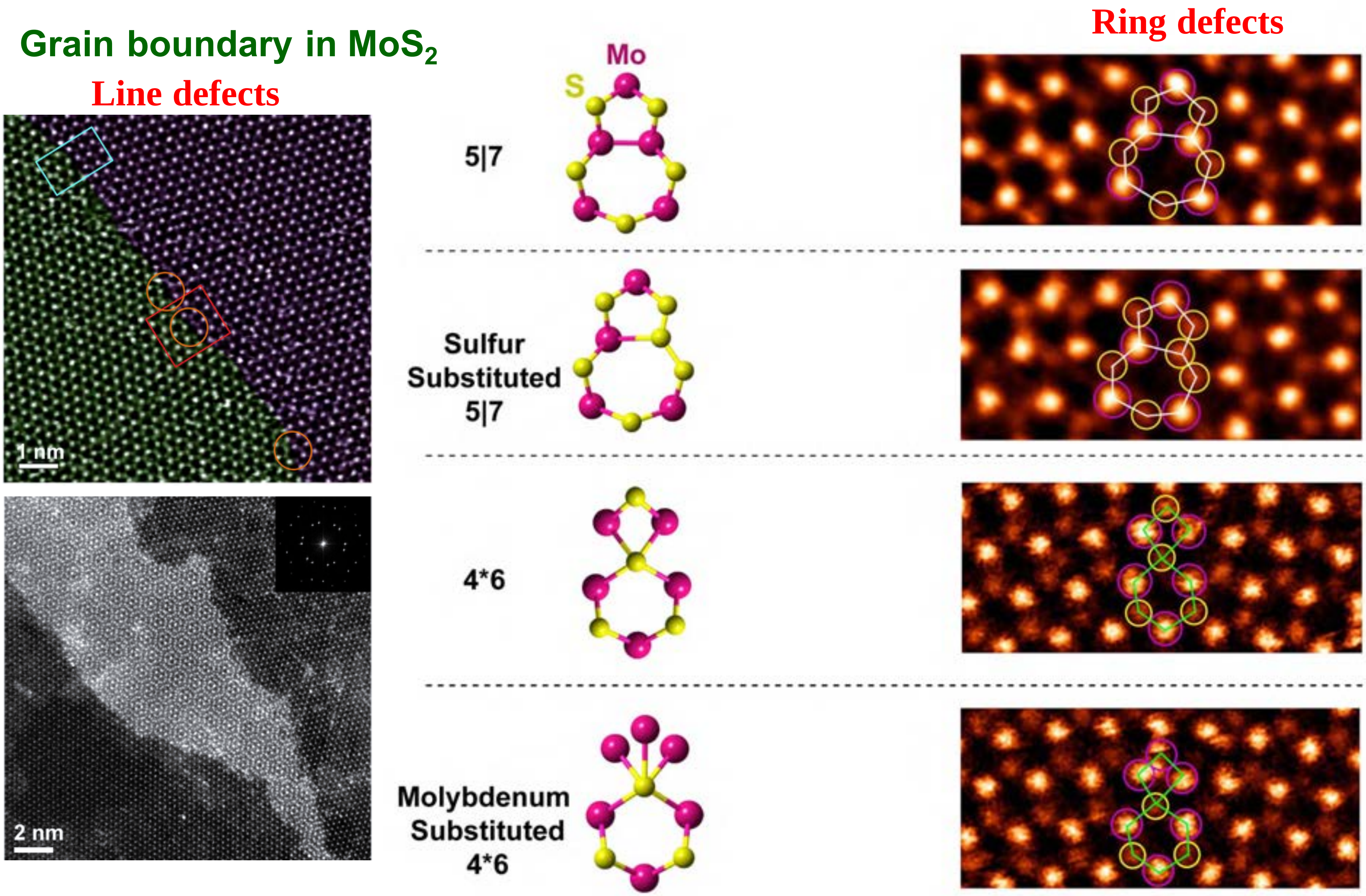




Terrones, H., Ruitao, Lv, Terrones, M., Dresselhauss, M,S. Reports on Progress In Physics, Vol. 75, 062501, 2012

Seifert, G., Terrones, H., Terrones, M., et al., Physical Review Letters, Vol. 85, 146(2000).

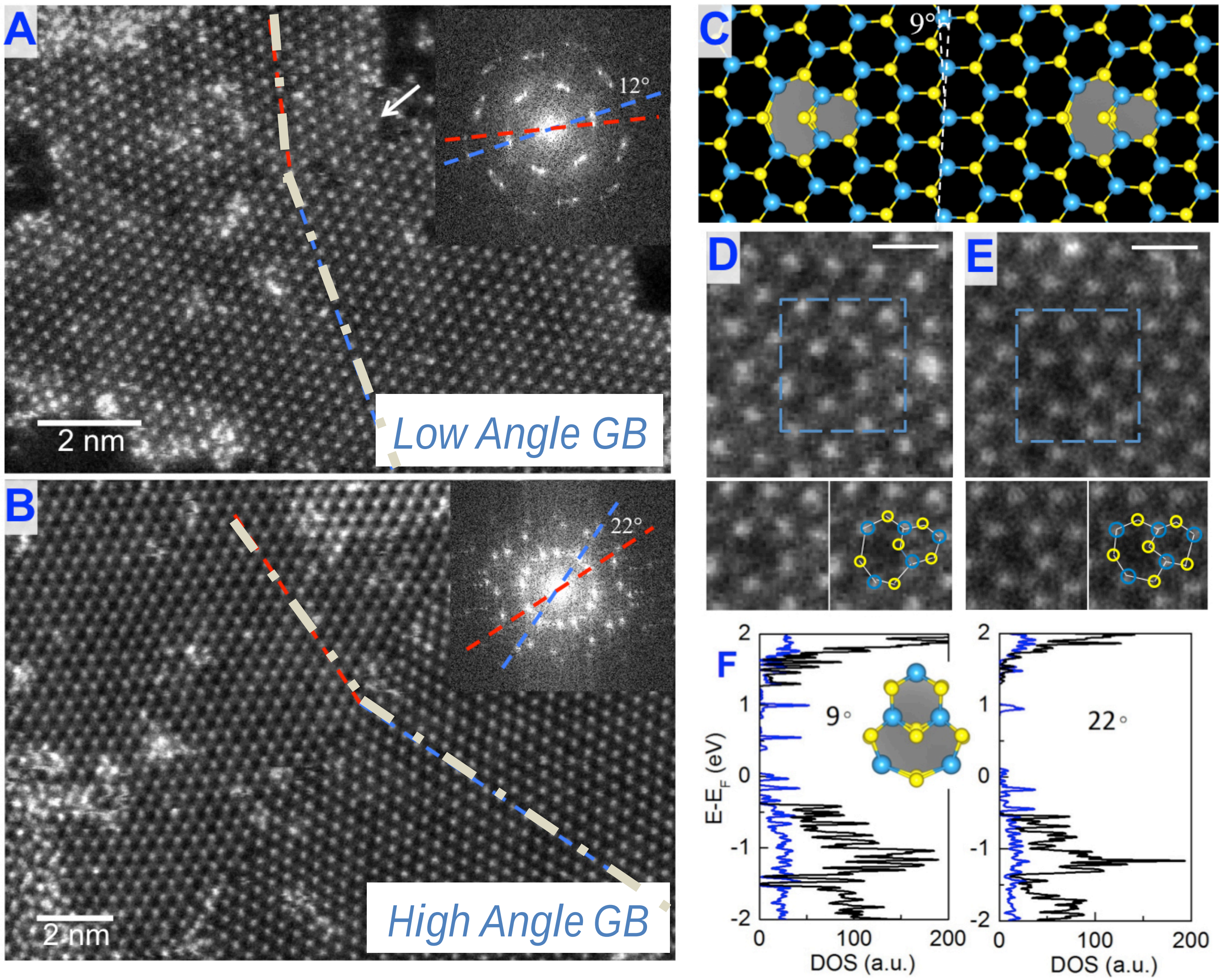
Synthesis and Characterization of MoS_2 layers



S. Najmaei, et al., Nature Materials (2013)

Grain Boundaries in WS_2 monolayers

In Collaboration with N. Alem, P. Ercuis (NCEM), A. Azizi, B. Yakobson

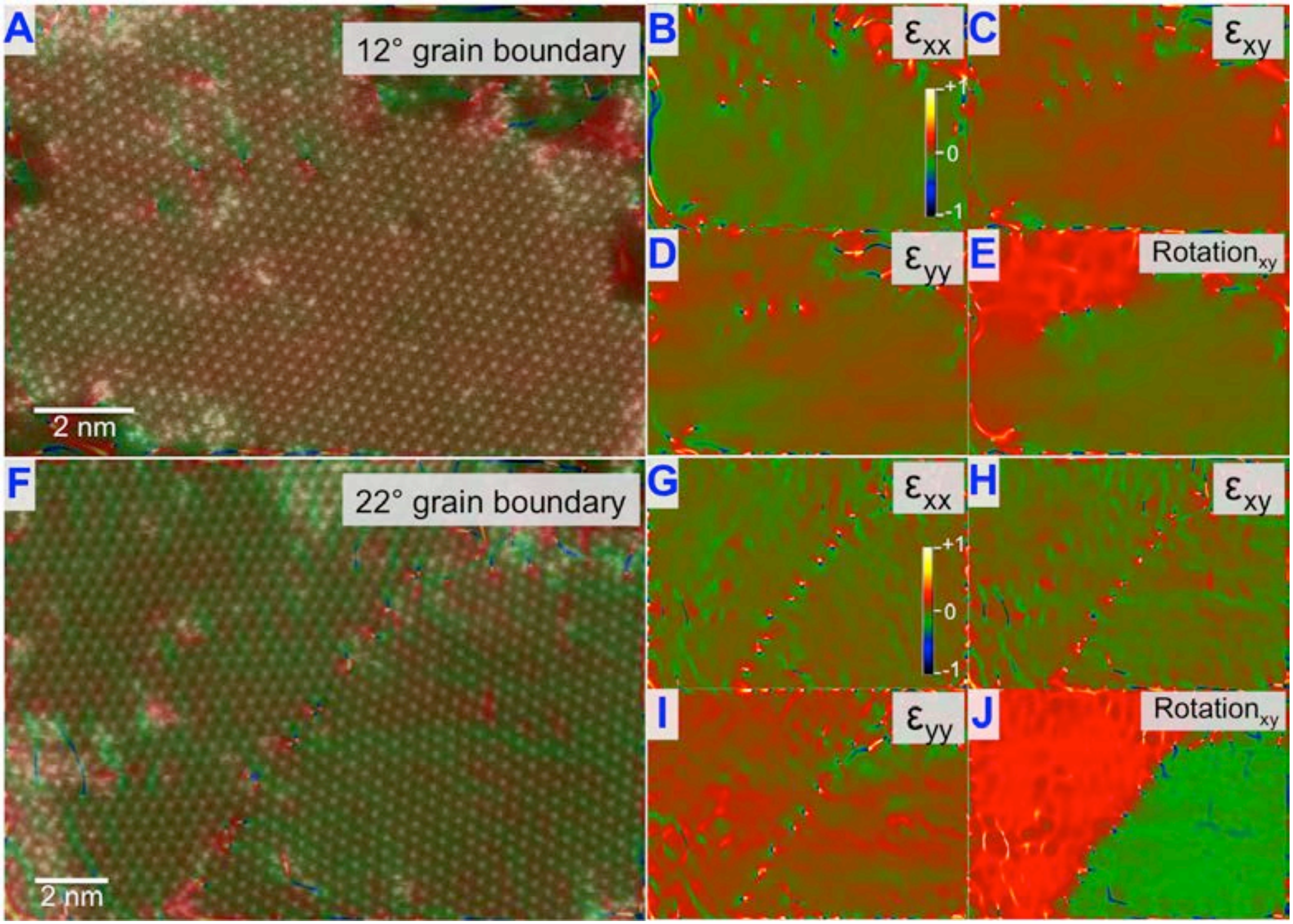


Dislocation Cores

A. Azizi, et al. Nature Communications 5, 4867 (2014)

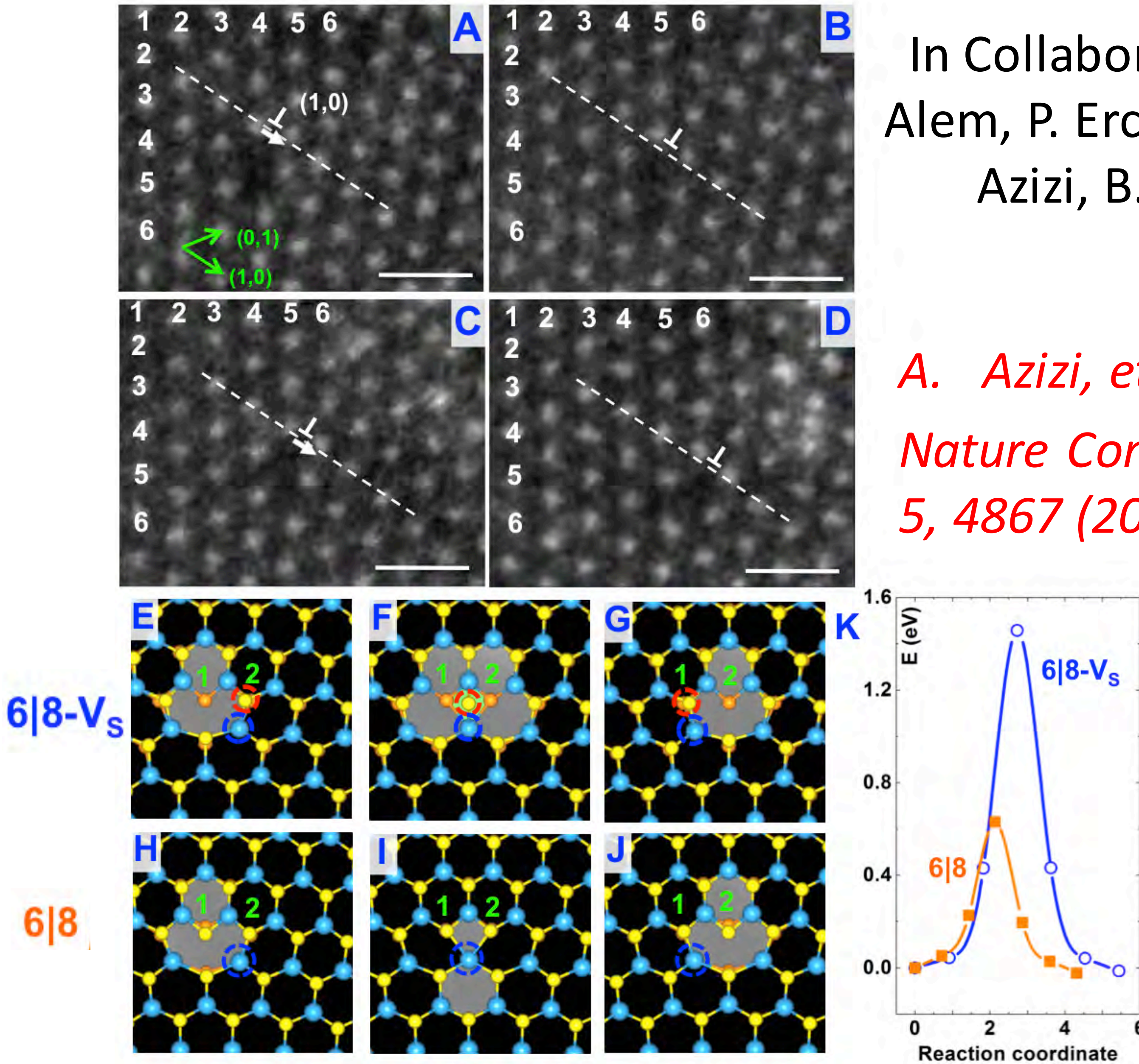
Strain Field Mapping in GB of WS_2

A. Azizi, et al. Nature Communications 5, 4867 (2014)



Using geometric phase analysis (GPA); see Ultramicroscopy 74, 131–146 (1998)

Dislocation Migration in GB of WS_2

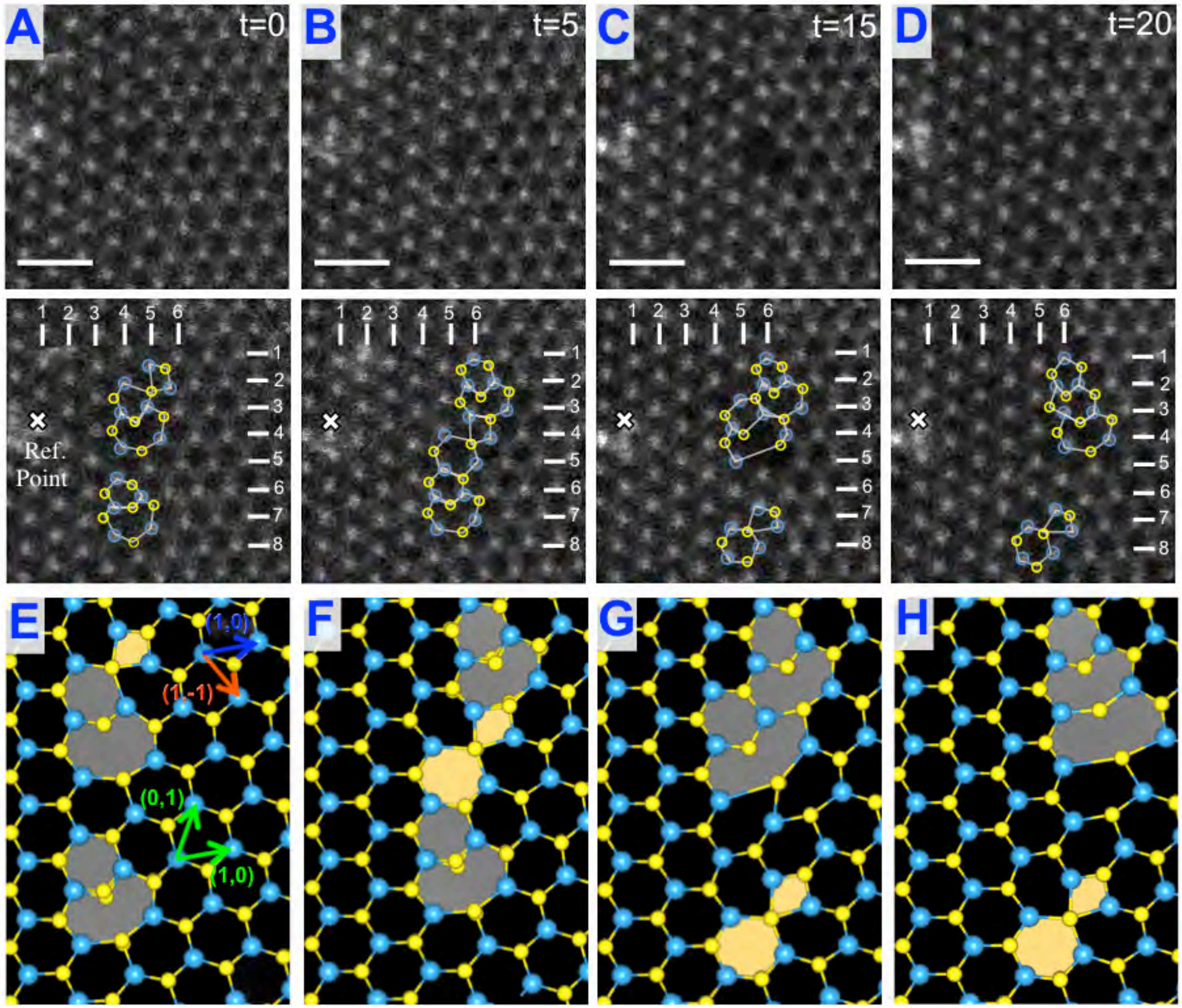


In Collaboration with N. Alem, P. Ercuis (NCEM), A. Azizi, B. Yakobson

A. Azizi, et al.

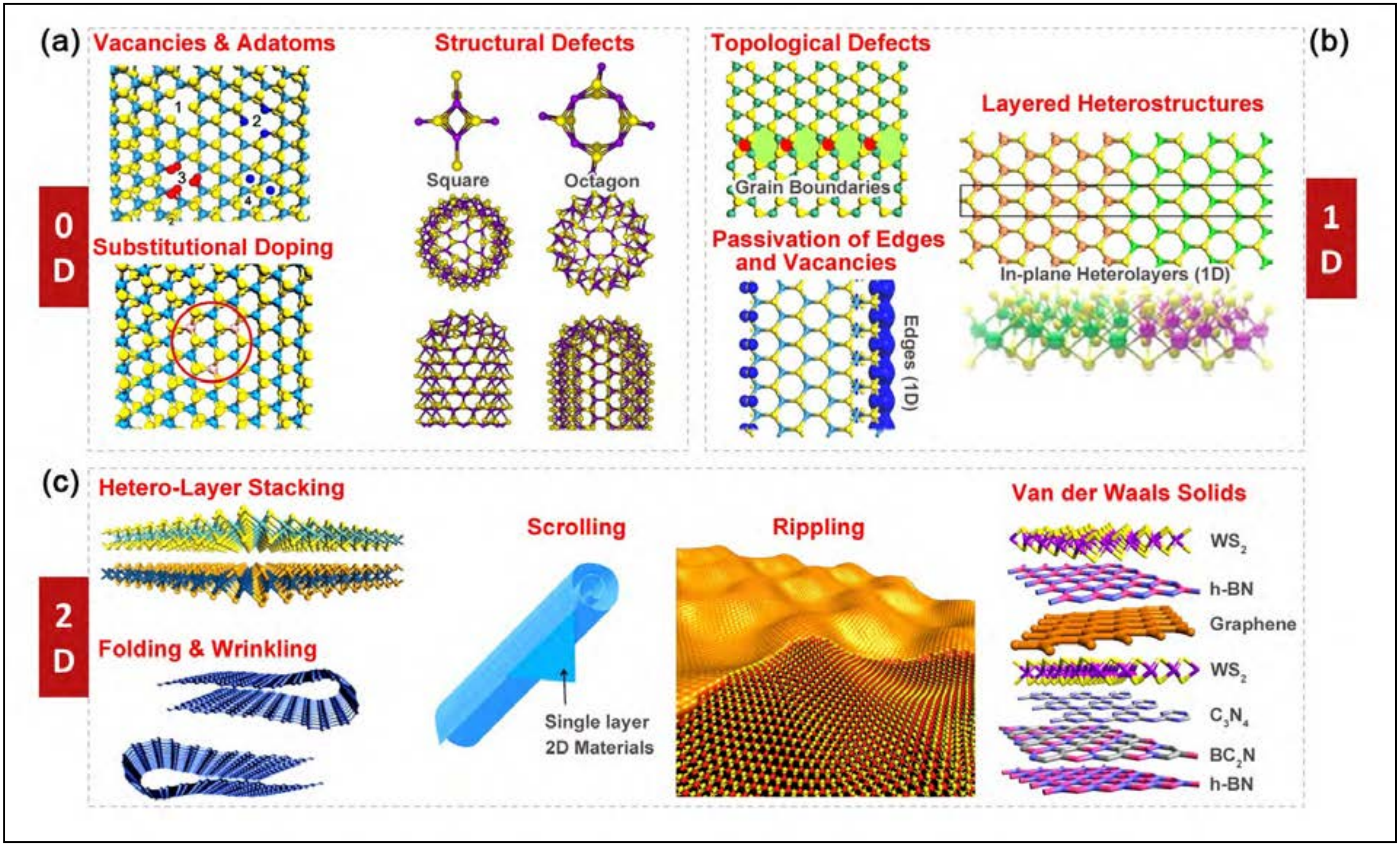
Nature Communications 5, 4867 (2014)

Dislocation Migration in GB of WS_2



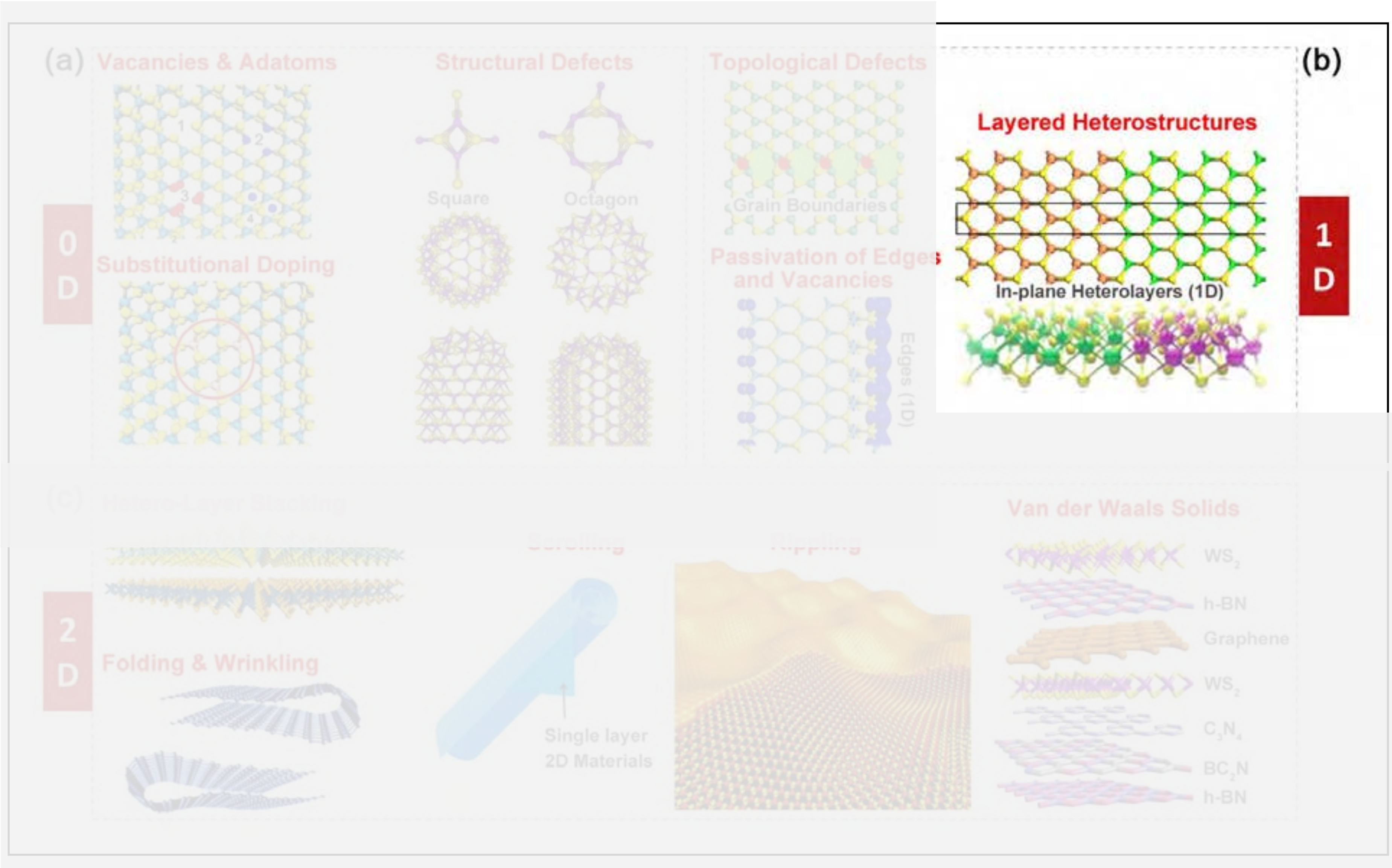
A. Azizi, et al. Nature Communications 5, 4867 (2014)

Defect Engineering



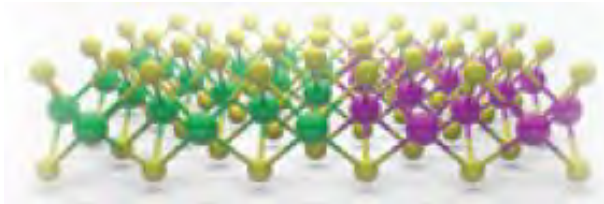
Z. Lin, B.R. Carvalho, E. Kahn, R. Lv, R. Rao, H. Terrones, M.A. Pimenta, M. Terrones. 2D Materials (2016)

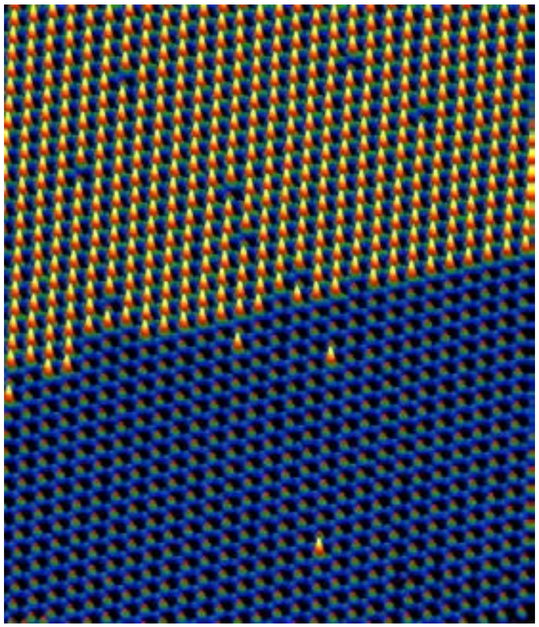
Defect Engineering



Z. Lin, B.R. Carvalho, E. Kahn, R. Lv, R. Rao, H. Terrones, M.A. Pimenta, M. Terrones. 2D Materials (2016)

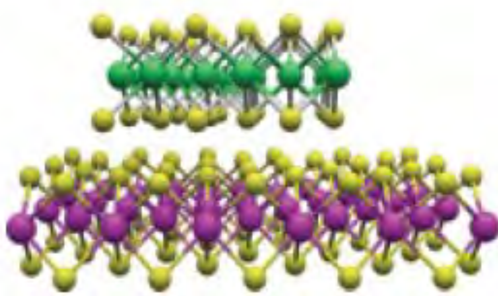
Bottom up synthesis of TMD heterostructures: Role of Te



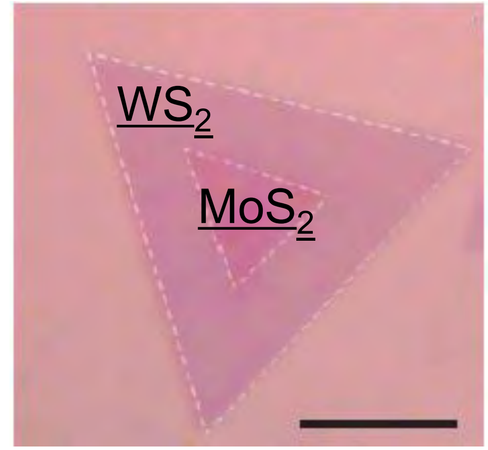


Phase Separation& Sharp Interface

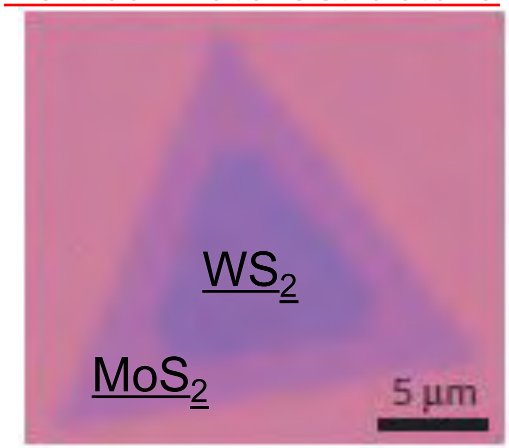
Lateral heterostructure	Central region	Peripheral region
MoS_2-WS_2	MoS_2	WS_2
$MoSe_2$-WSe_2	$MoSe_2$	WSe_2
MoS_2-$MoSe_2$	MoS_2	$MoSe_2$
WS_2-WSe_2	WS_2	WSe_2
Vertical heterostructure	**Bottom layer**	**Top layer**
MoS_2-WS_2	MoS_2	WS_2



Lateral heterostructure

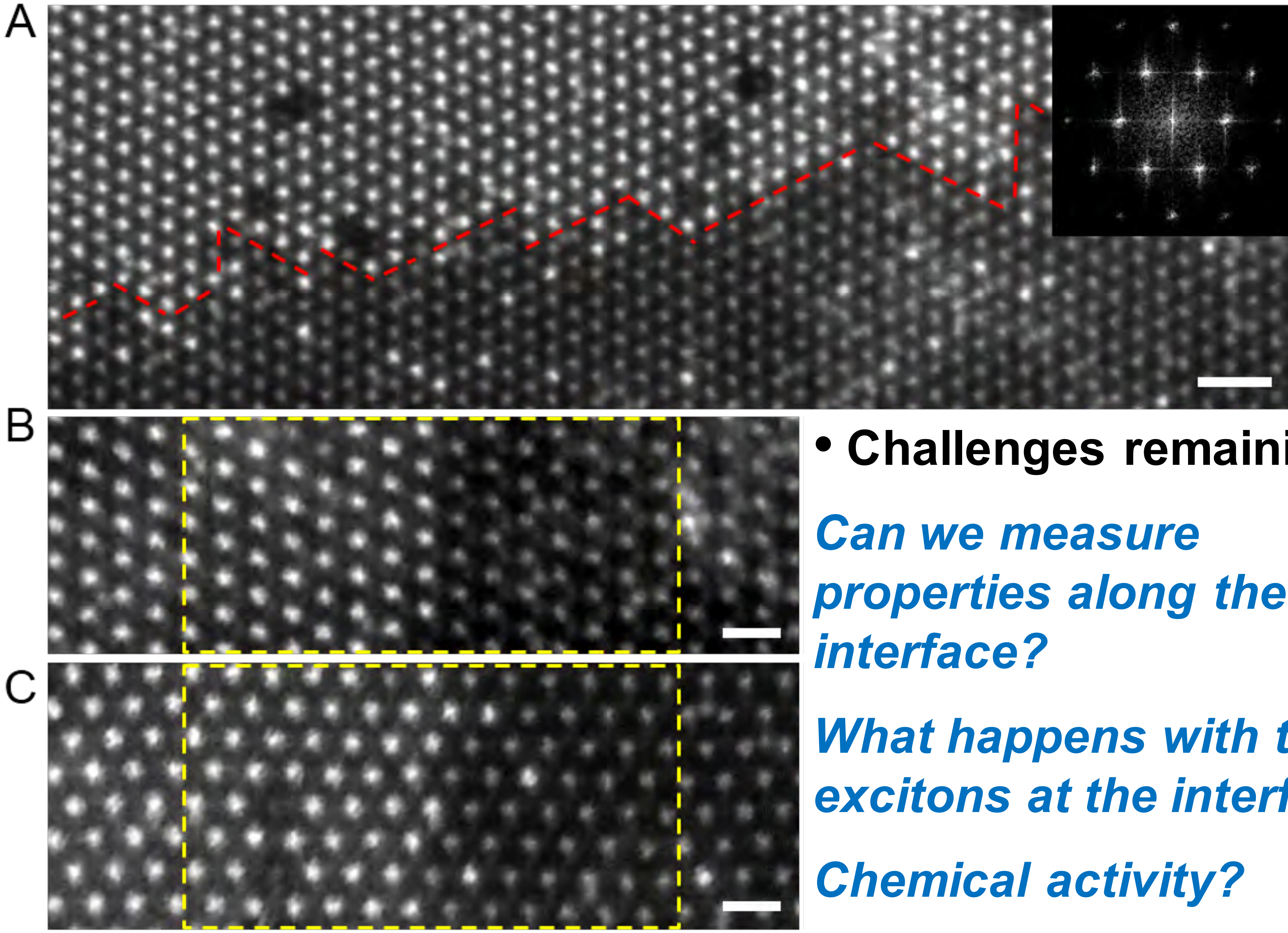


Vertical heterostructure



Gong, et al. Nat. Mater. doi: 10.1038/nmat4091
Duan, et al. Nat. Nano. doi: 10.1038/nnano.2014.222
Huang,et al. Nat. Mater. doi: 10.1038/nmat4064

Large Scale Synthesis of MoS_2/WS_2 In-plane Heterostructures



- **Challenges remaining**

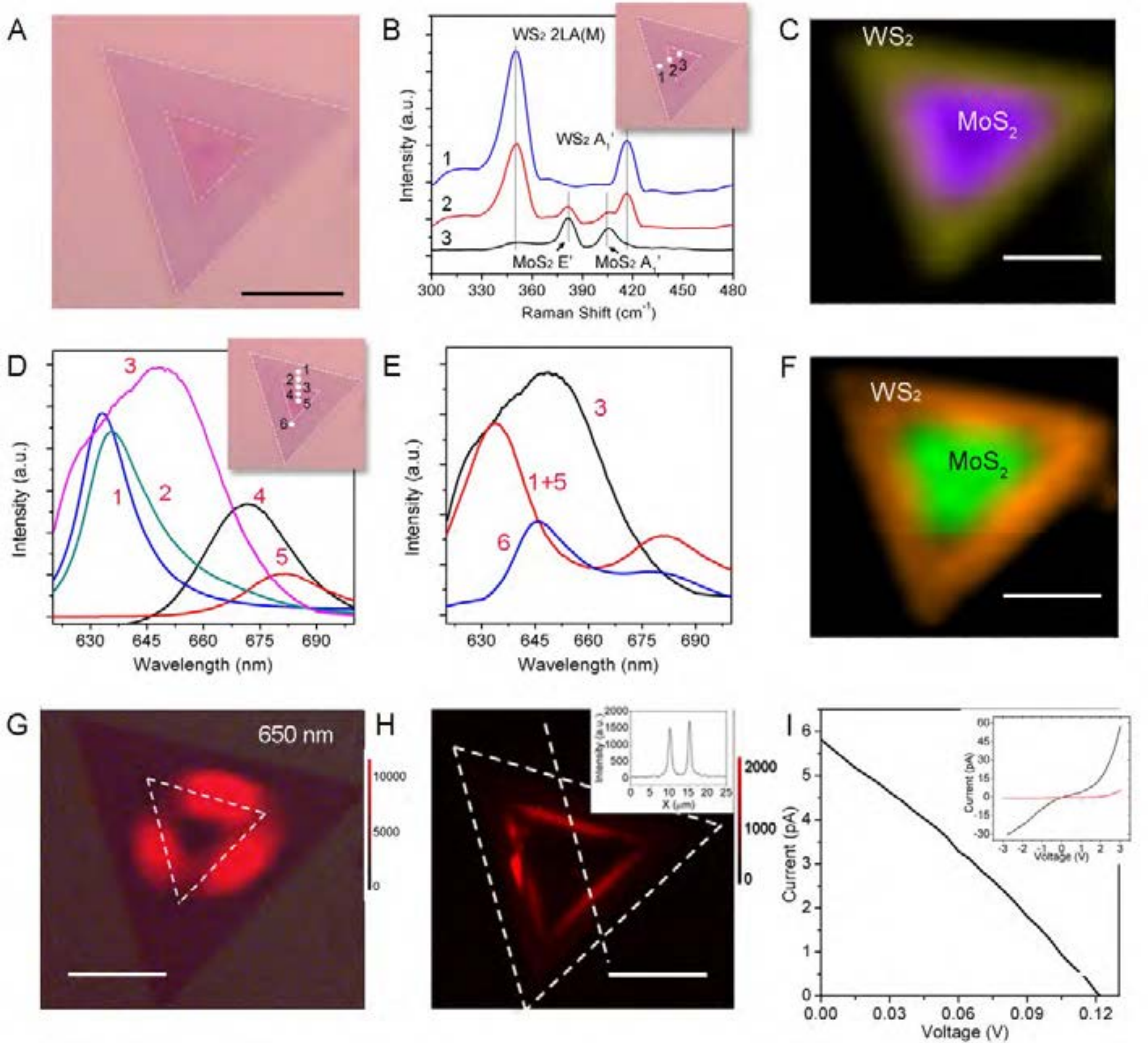
Can we measure properties along the interface?

What happens with the excitons at the interface?

Chemical activity?

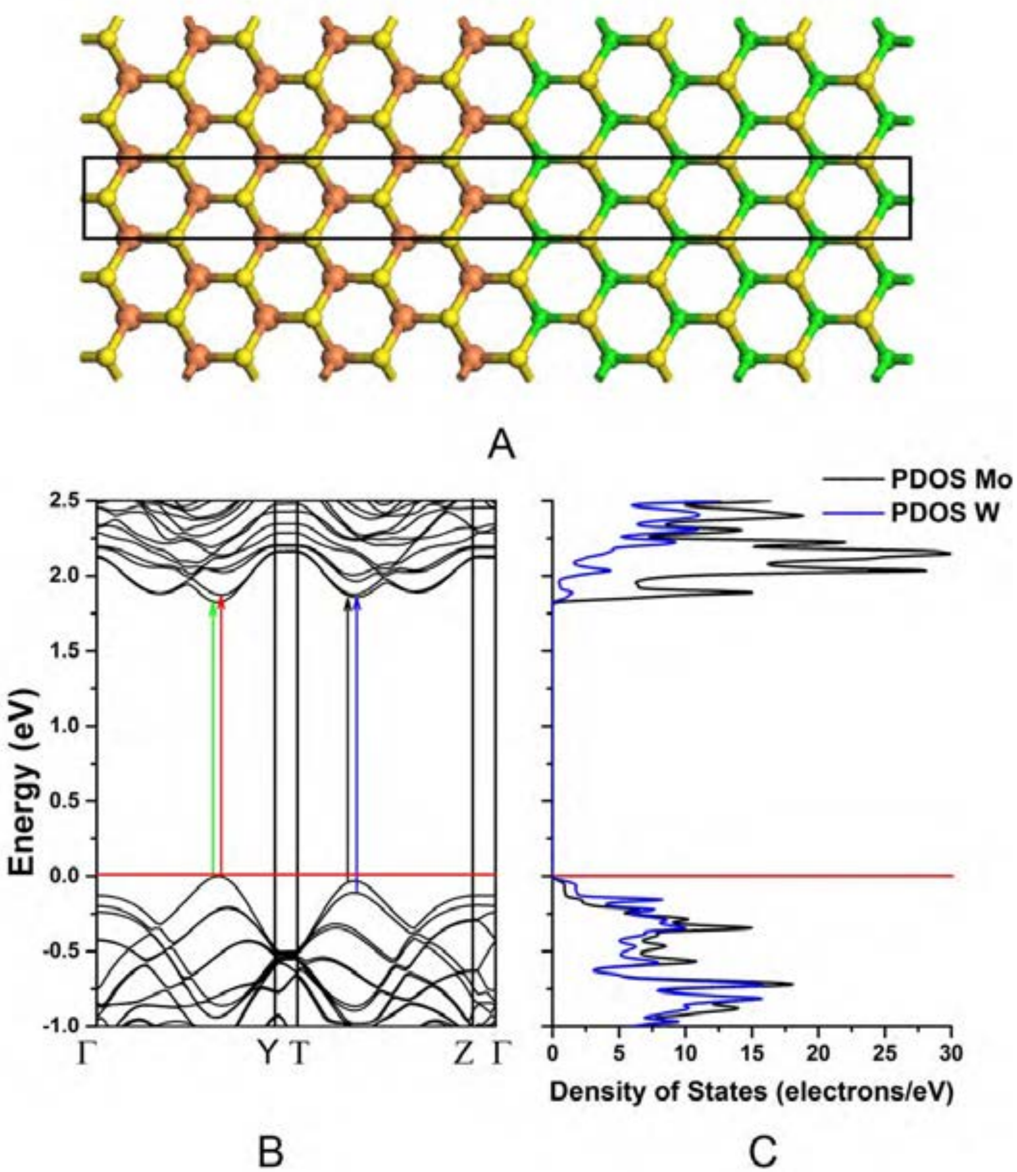
Gong, et al. Nature Materials (2014). Collaboration with P.M. Ajayan, J. Lou

Large Scale Synthesis of MoS_2/WS_2 In-plane Heterostructures



Gong, et al. Nature Materials (2014). Collaboration with P.M. Ajayan, J. Lou

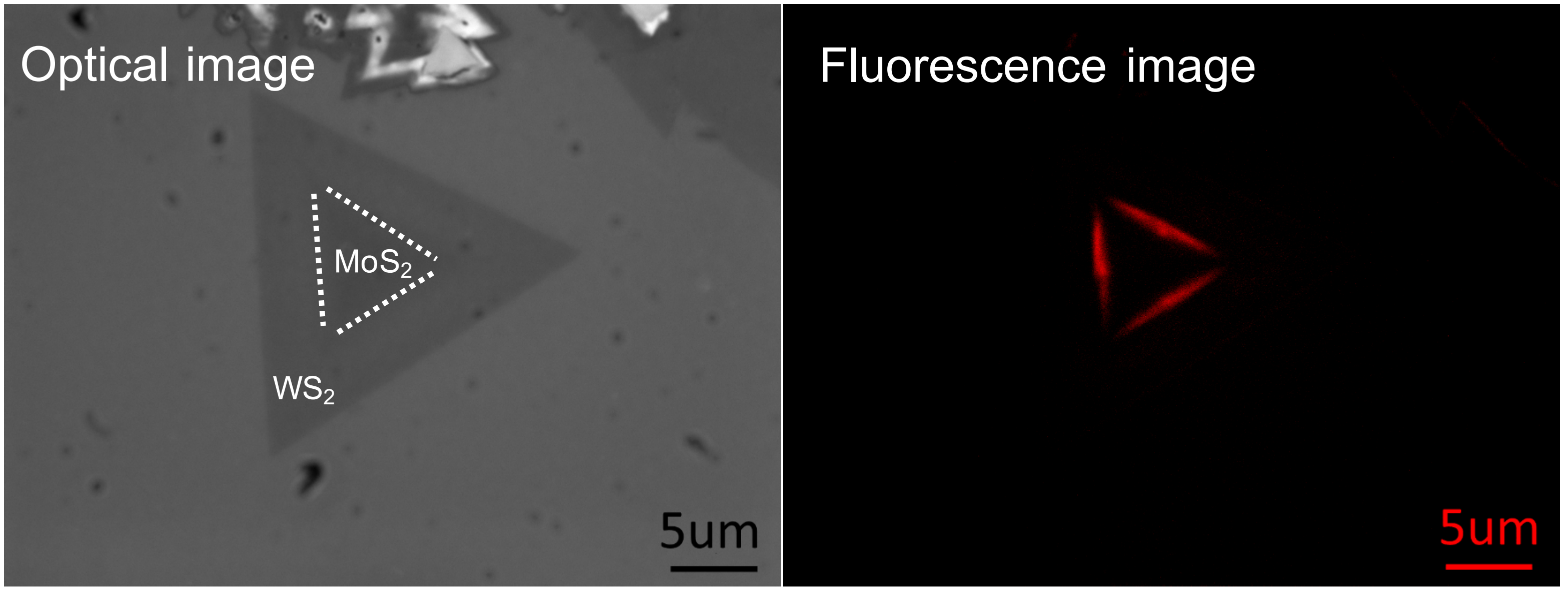
Large Scale Synthesis of MoS_2/WS_2 In-plane Heteroetrcutures

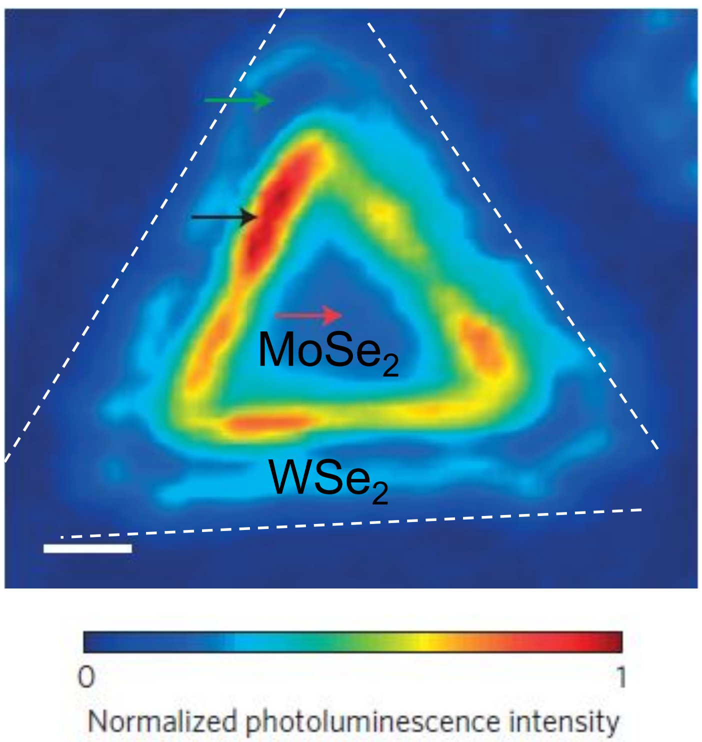


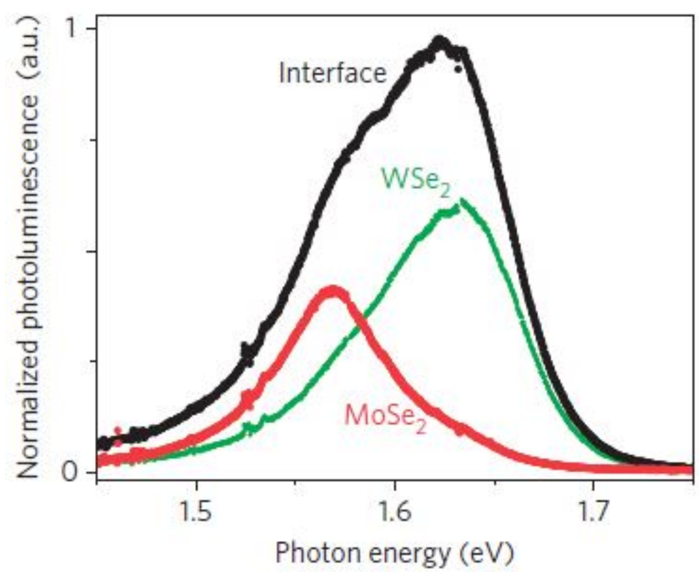
***(B)** Band structure of the cell in (A) showing direct transitions at 1.825 eV (679 nm. Green arrow), 1.875 eV (661.33 nm. Red arrow), 1.889 eV (656.43 nm. Black arrow), 1.908 eV (649.89 nm. Not shown), 1.968 eV (630.08 nm. Blue arrow), 1.987 eV (624.05 nm. Not shown).*

Gong, et al. Nature Materials (2014). Collaboration with P.M. Ajayan, J. Lou

Enhanced radiative recombination at interfaces

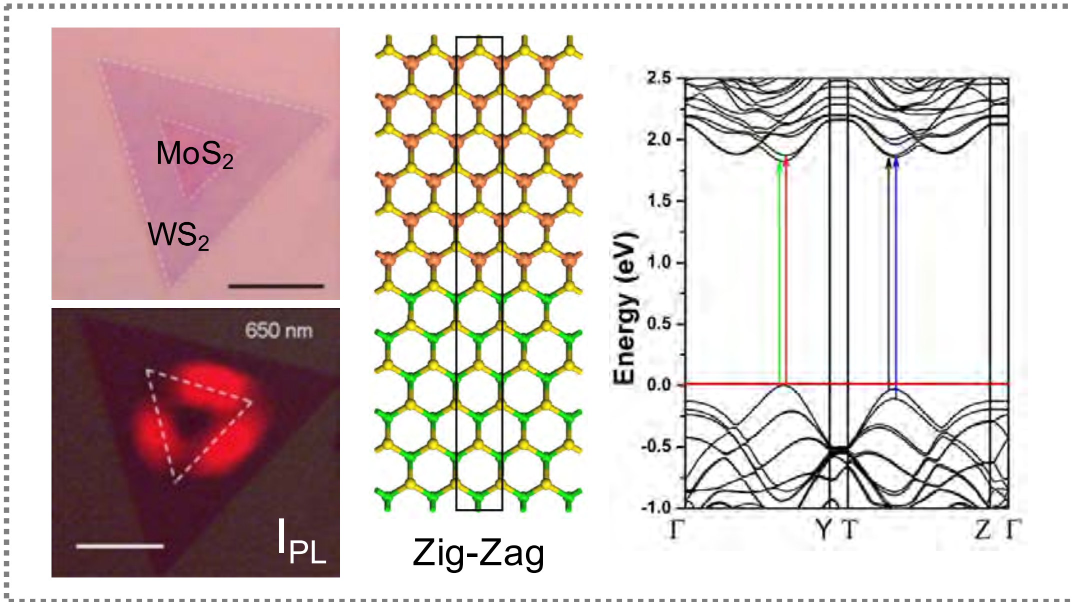


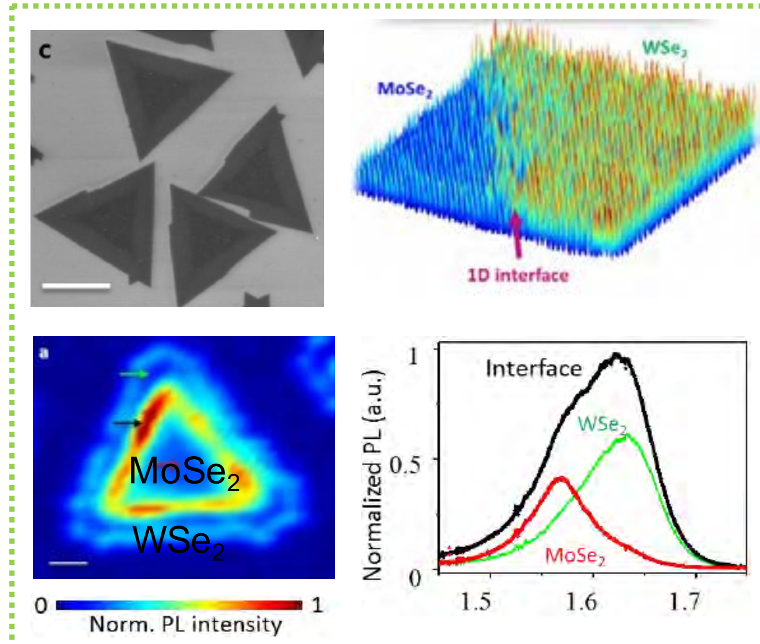


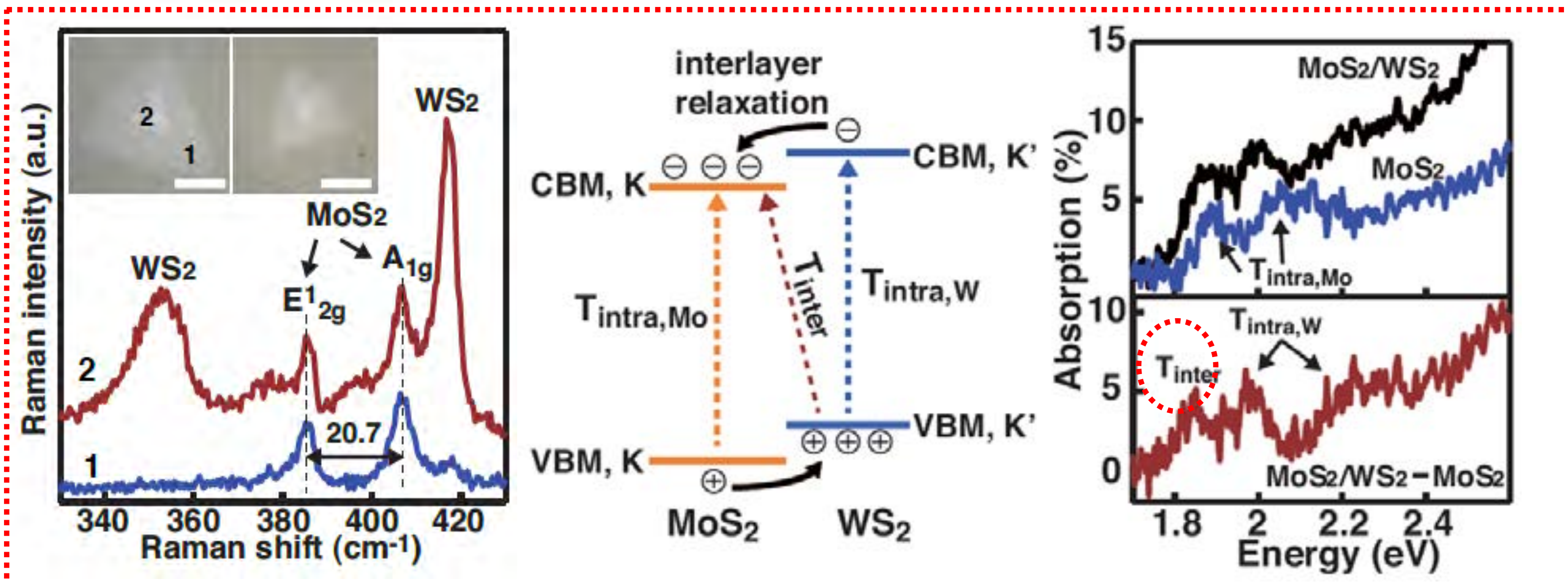


Lin, Gong, et al. unpublished
Gong, et al. Nat. Mater. ***13*** *1135 (2014).*
Huang, et al. Nat. Mater. DOI: 10.1038/NMAT4064.

Novel excitons in heterostructured TMDs
----lateral and vertical structures







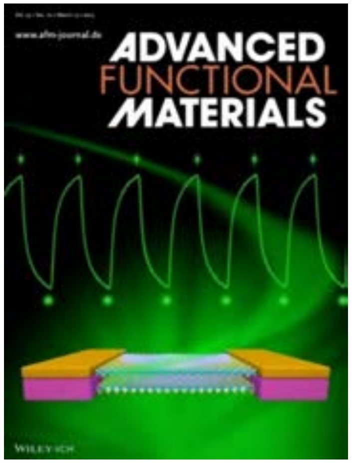
Gong, et al. under review. Yu, et al. arXiv:1403.6181. Huang, et al. arXiv:1406.3122.

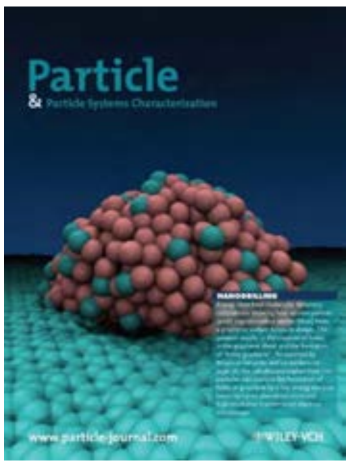
WE THANK

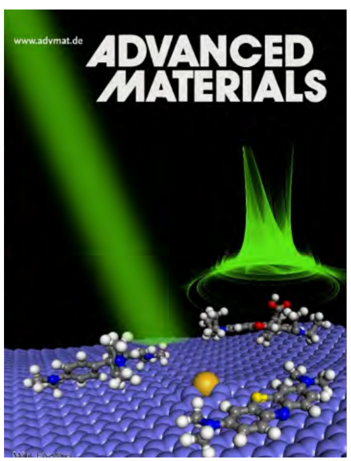
ARO MURI W911NF-11-1-0362: Atomic Layers of Nitrides, Oxides, and Sulfides (ALNOS)

AFOSR MURI FA9550-12-1-0035: Synthesis and Characterization of 3D Carbon Nanotube Solid Networks

Penn State Center for Nanoscale Science







ACCOUNTS of chemical research

The Rise of Two-Dimensional Materials