MOCVD Routes to 2D Crystals

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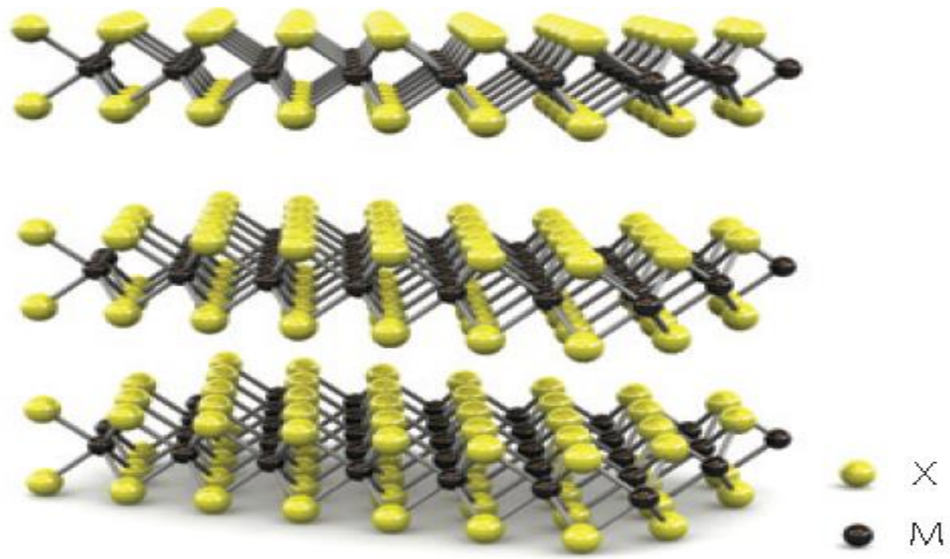
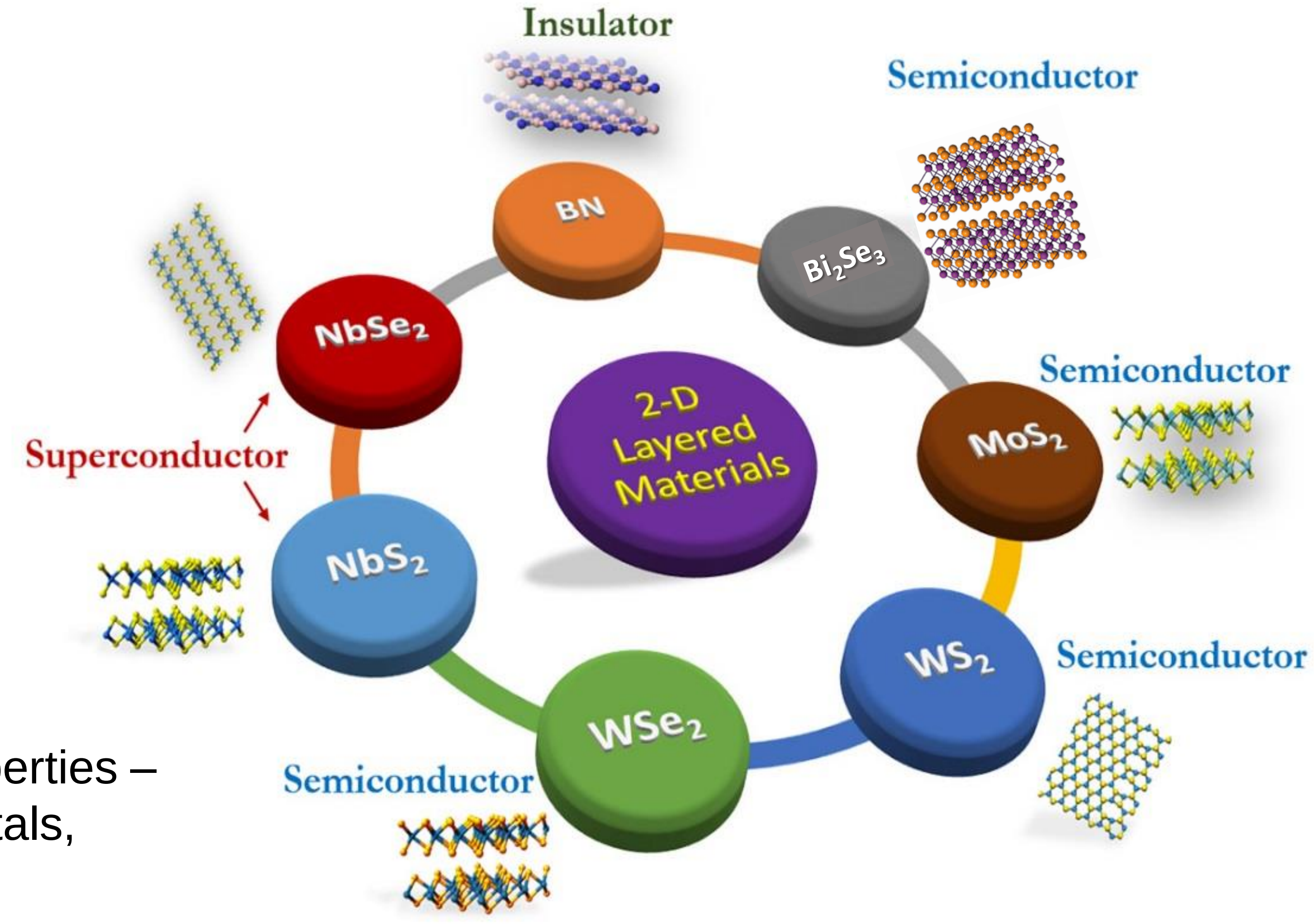
Layered Materials



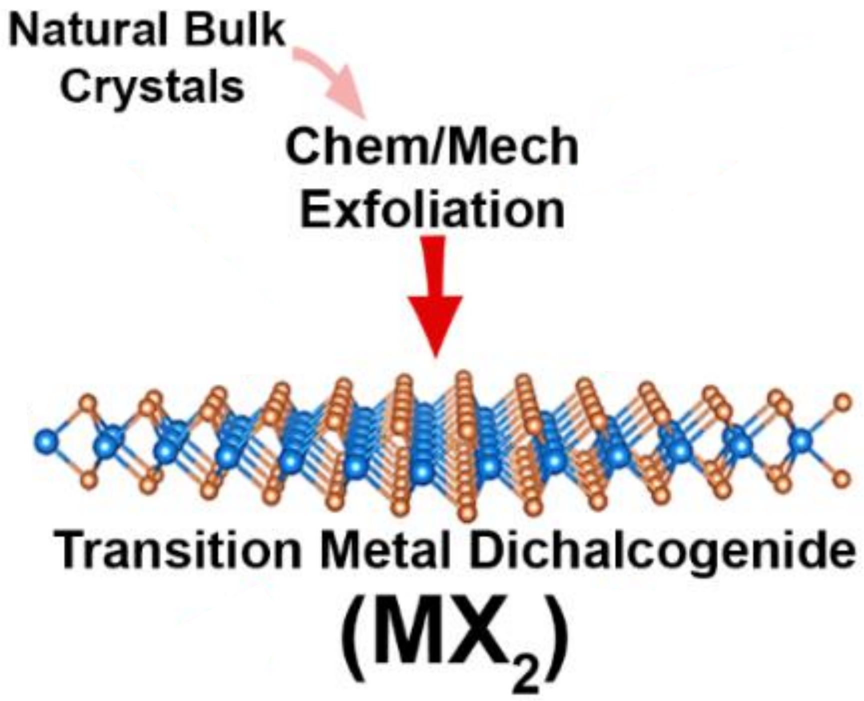
Q.H. Huang, et al.
Nature Nanotech. 7 (2012) p. 699



- Graphene-like layered materials
- Exhibit wide variety of electronic properties – insulators, semiconductors, semi-metals, superconductors

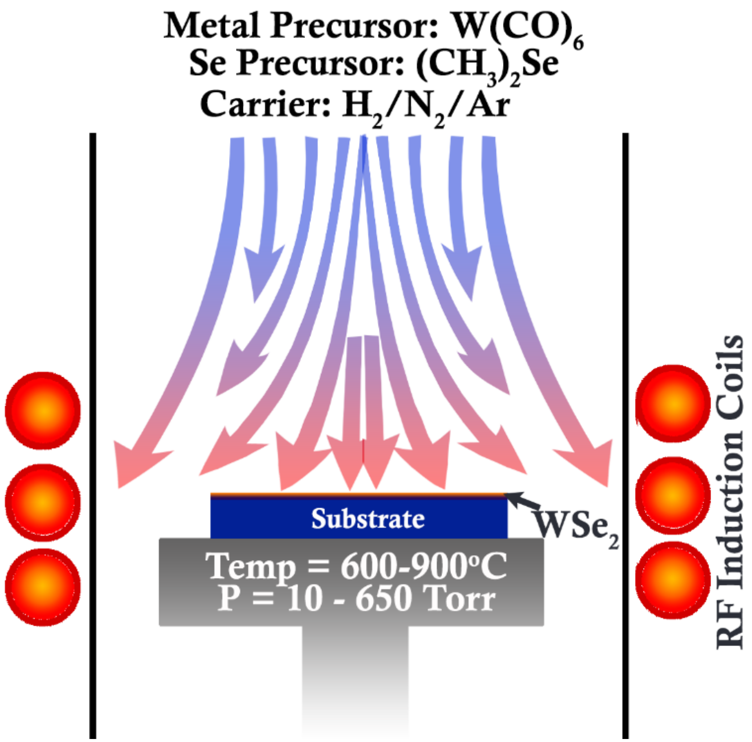
The TMD Synthesis "Atlas"

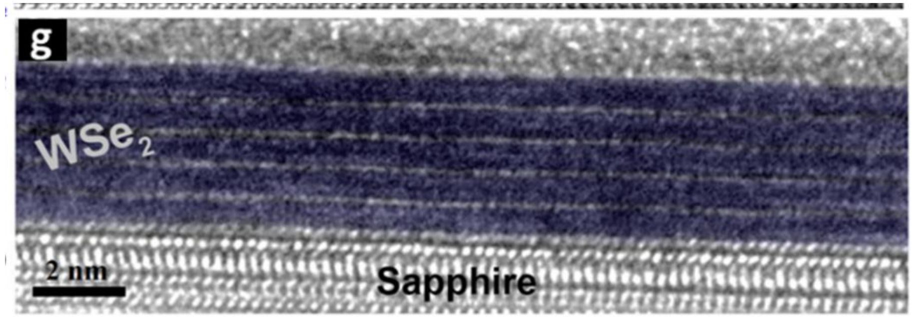
S. Das, J.A. Robinson, M. Terrones, et al.
Annual Review of Materials Research, *45* , 1-27 (2015)

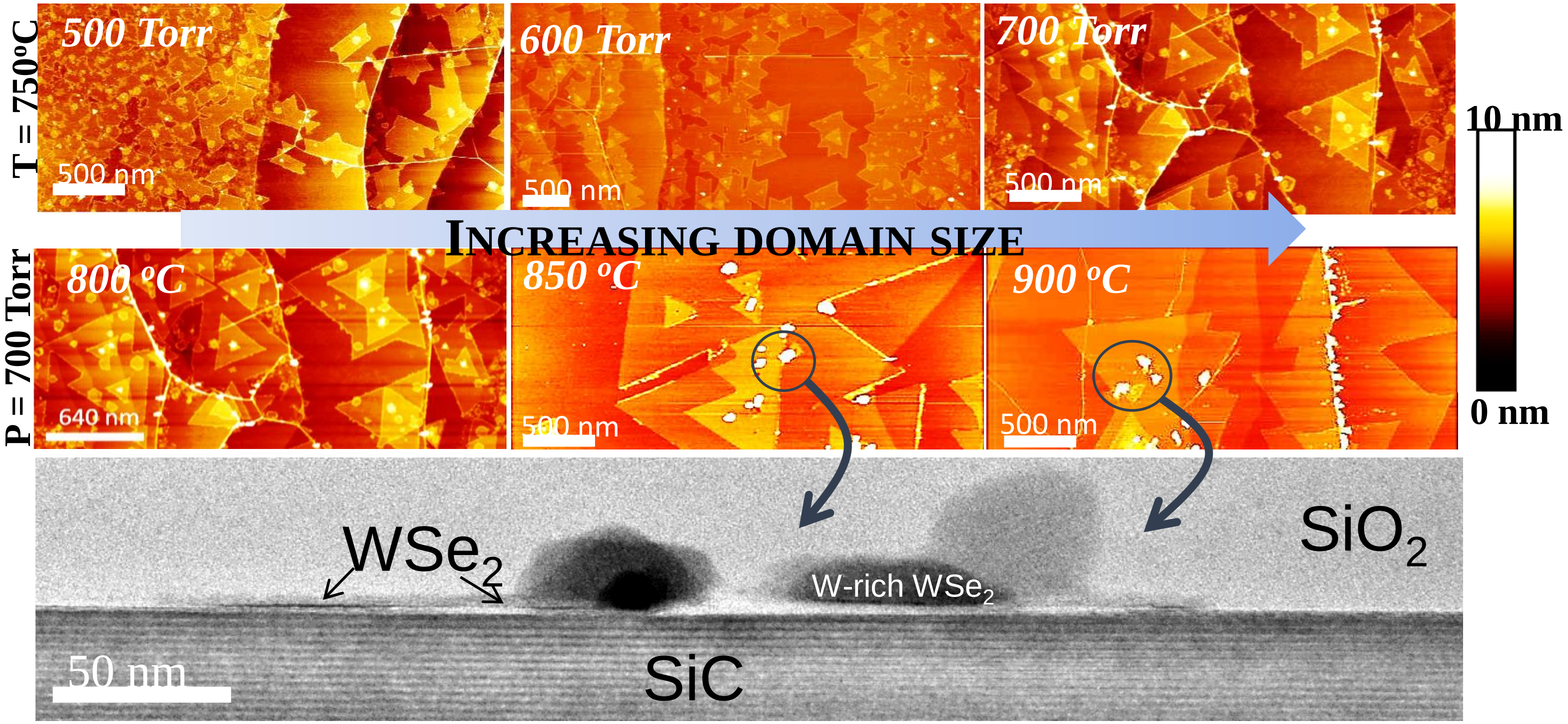


Tungsten Diselenide (WSe_2)

Metalorganic Chemical Vapor Deposition







- Highly scalable process
- Excellent control over W:Se ratio

S.M. Eichfeld, J.M. Redwing, J.A. Robinson, et al., ACS Nano, 2015, 9 (2), pp 2080–2087

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Tungsten Diselenide (WSe_2)

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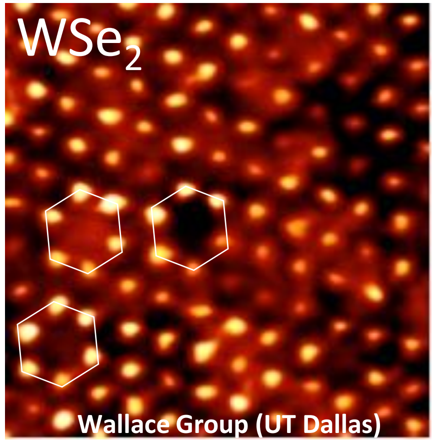
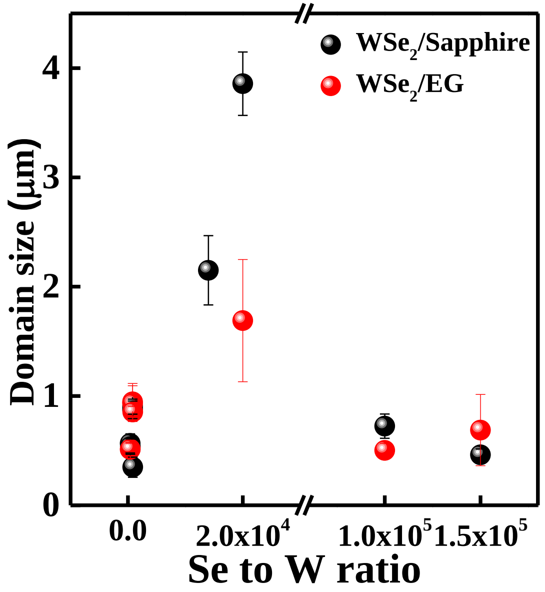
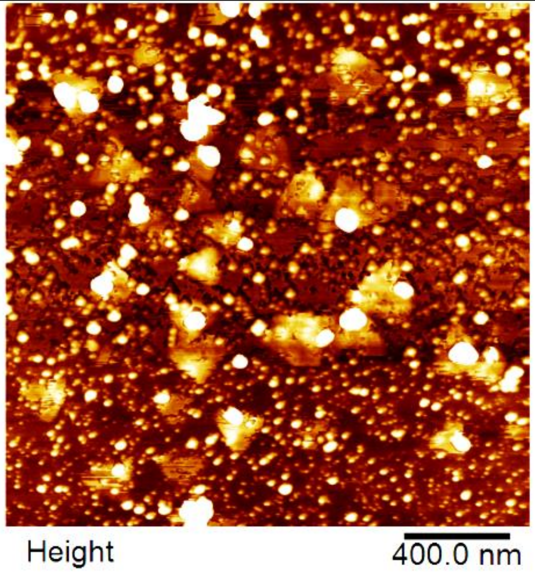


- Defects serve as nucleation sites in 2D materials.
- Typical defects are chalcogen (S,Se,Te) vacancies.

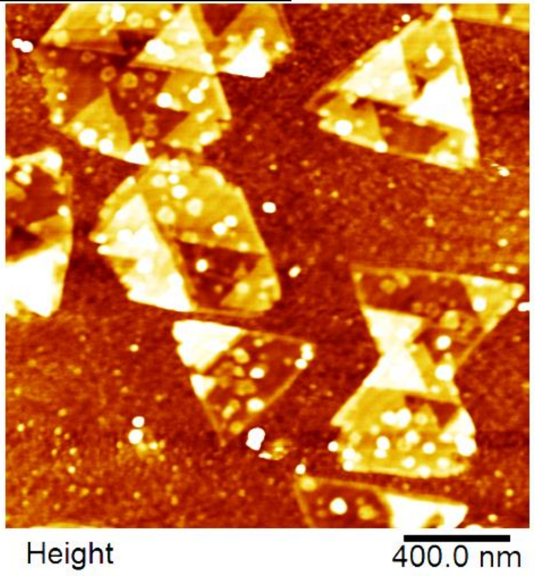


Se:W ratio has significant impact on domain size, shape, and “defect” formation

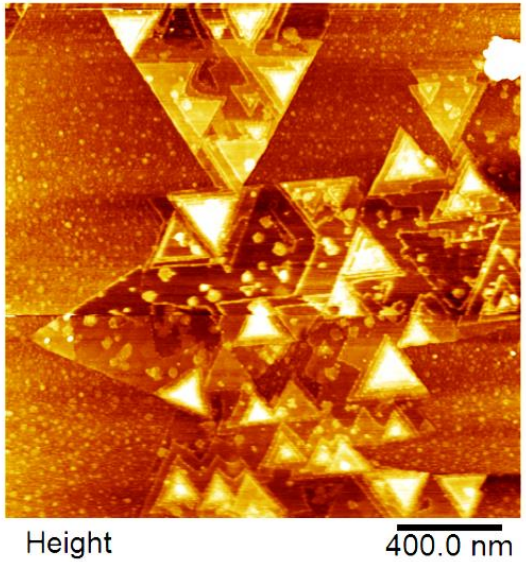
Temp (°C)	Time (min)	Pre- Anneal	Pressure (Torr)
800	30	500C, 15min	700



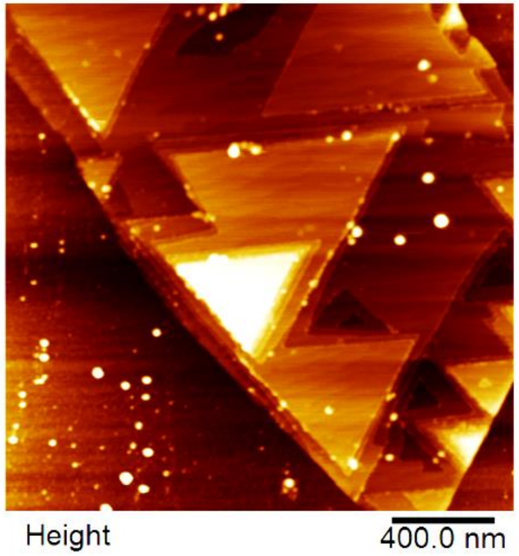
Se:W Ratio: 170

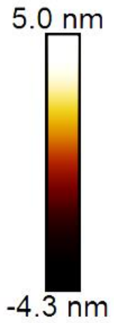


Se:W Ratio: 400



Se:W Ratio: 800





Se:W Ratio: 14000

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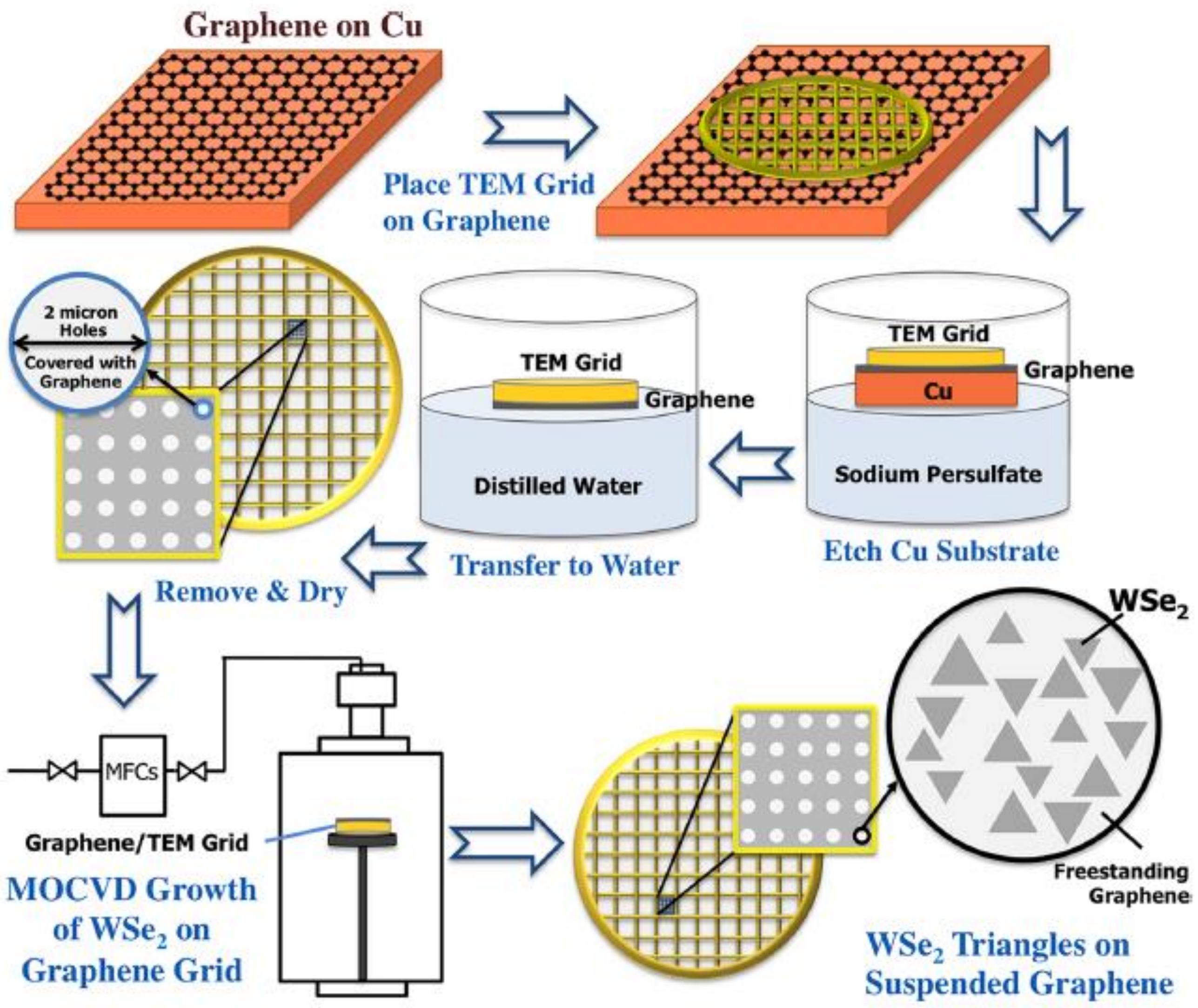
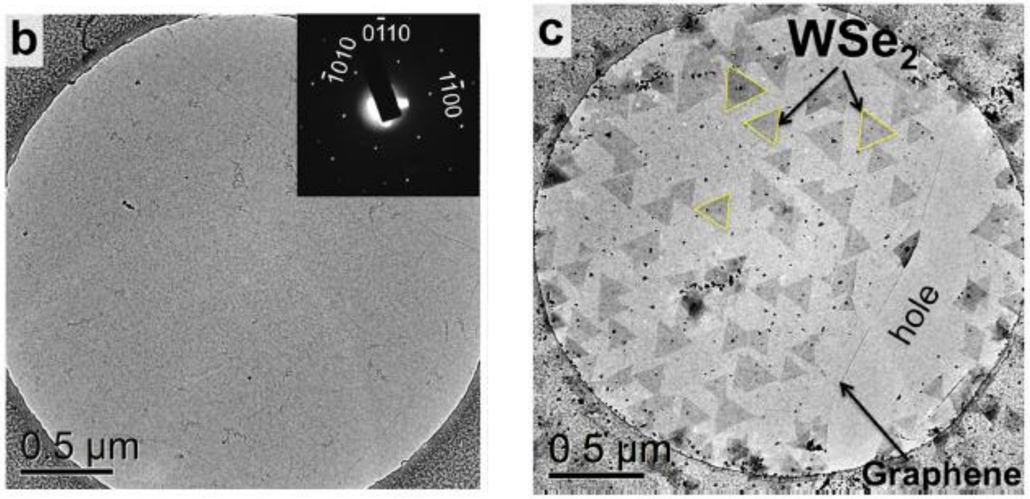
WSe_2 on Free Standing Graphene Templates



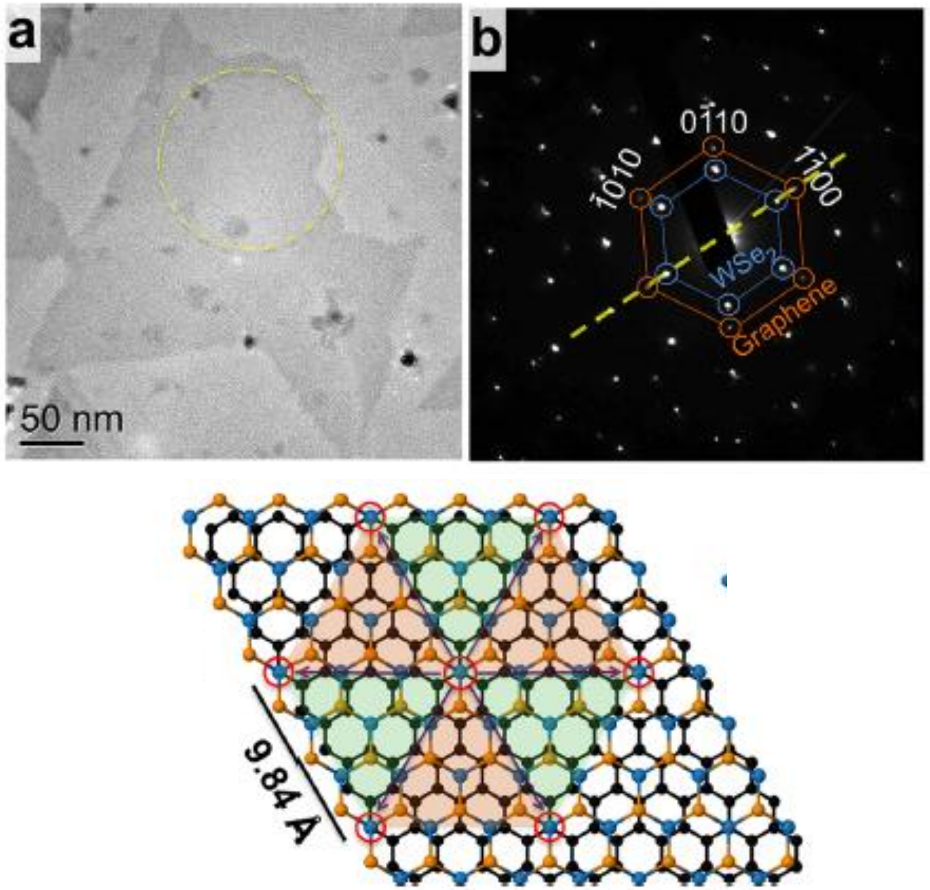


As Prepared　　　After MOCVD Growth

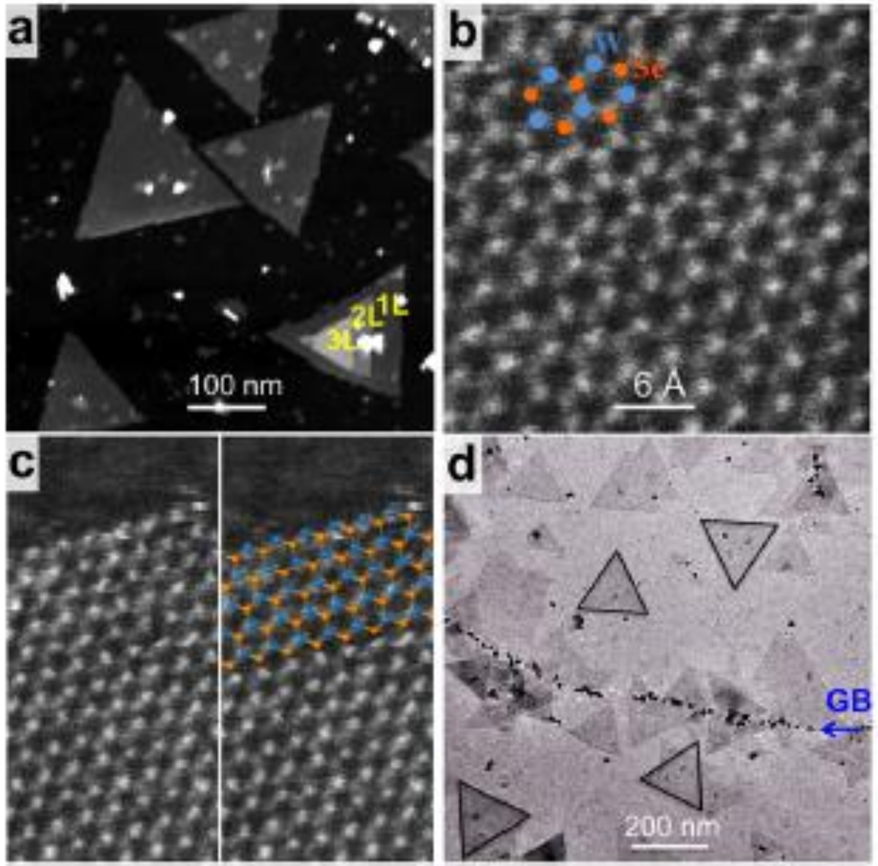
- Developed process to produce freestanding van der Waals heterostructures
- Ideal for investigating layer-layer interaction with graphene

A. Azizi, N. Alem, et al. ACS Nano 9 (2015) 4882.

WSe_2 – Epitaxy and Defects



(a) TEM image and (b) SAD pattern showing epitaxial relationship between WSe_2 and graphene
(c) Structural model showing alignment of W atoms in WSe_2 and C atoms in graphene (circled in red)

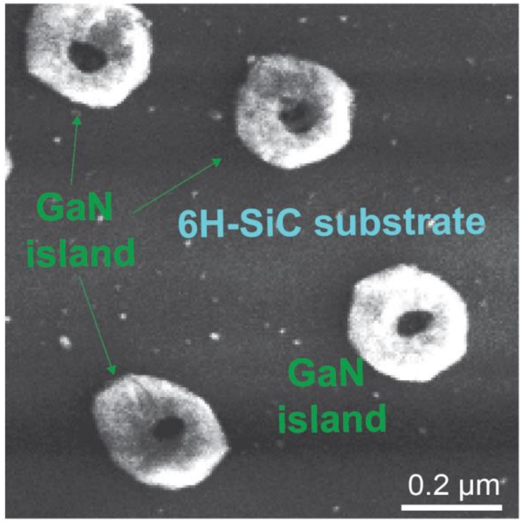


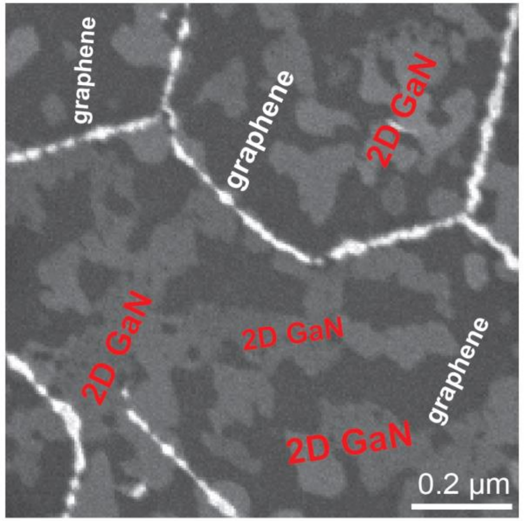
(a) HAADF-STEM image of monolayer and multilayer WSe_2
HAADF-STEM images of (b) monolayer WSe_2 and (c) edge region showing W-termination
d) TEM image showing nucleation near grain boundary in graphene

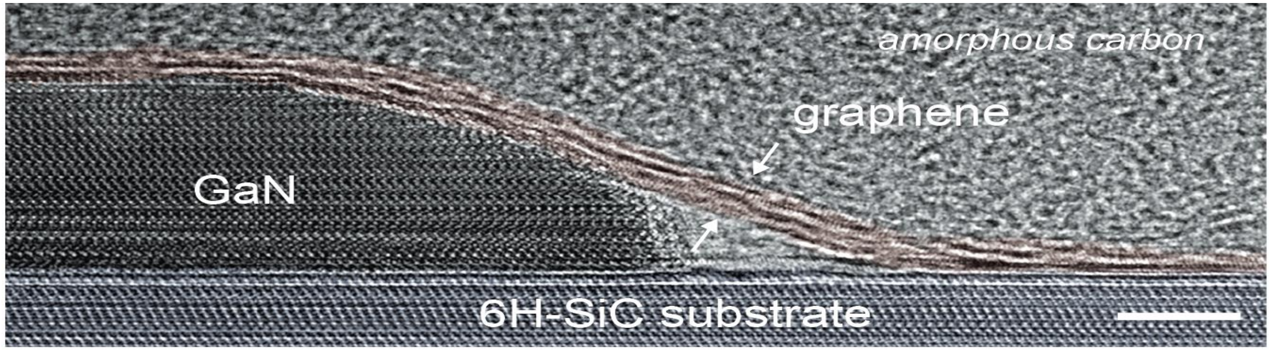
Pulsed MOCVD growth of GaN

SiC Substrate

Epitaxial Graphene

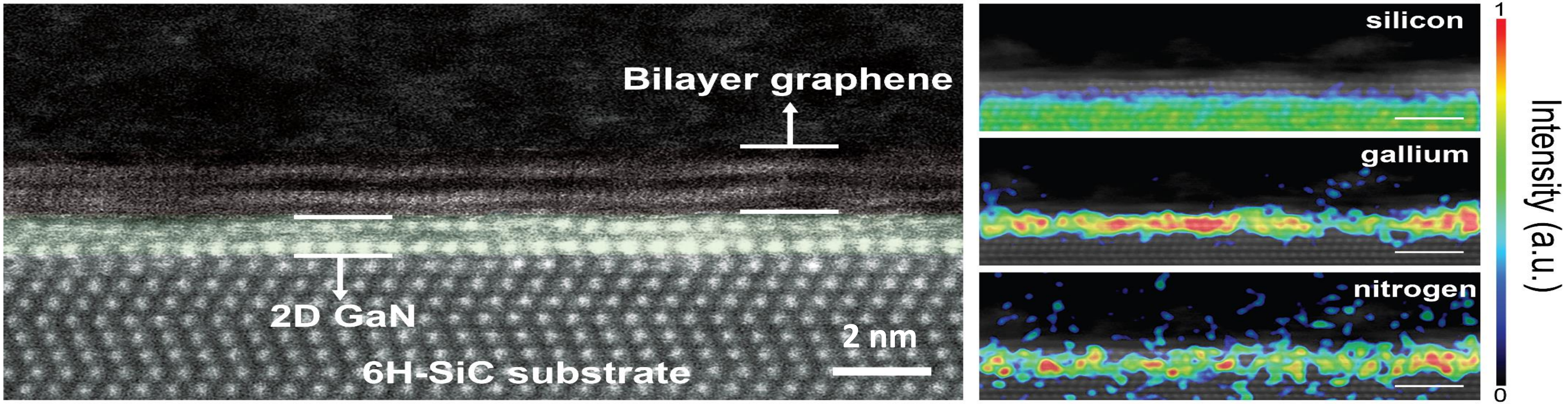




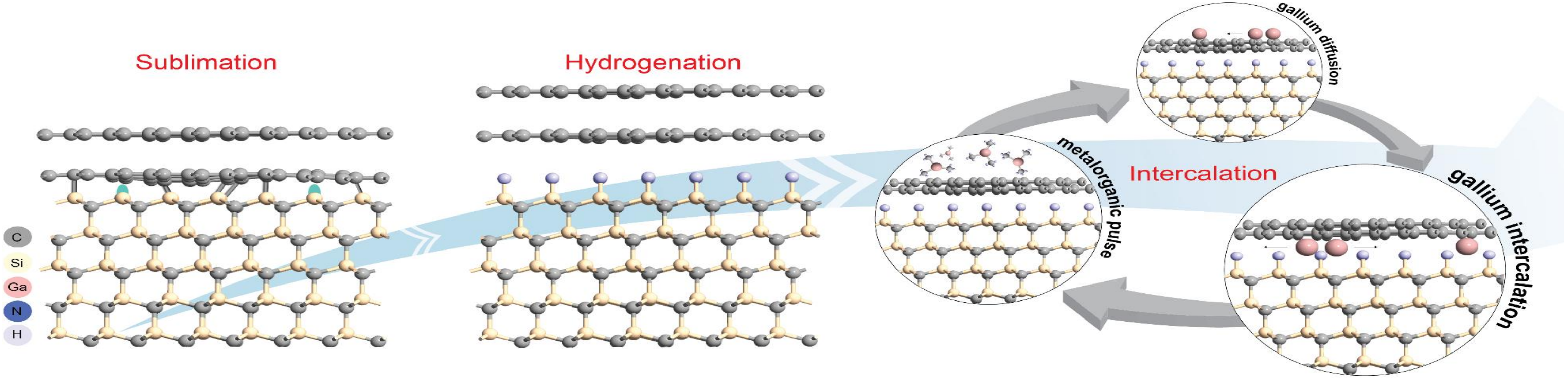


Cross-section TEM of GaN growing between graphene and SiC substrate

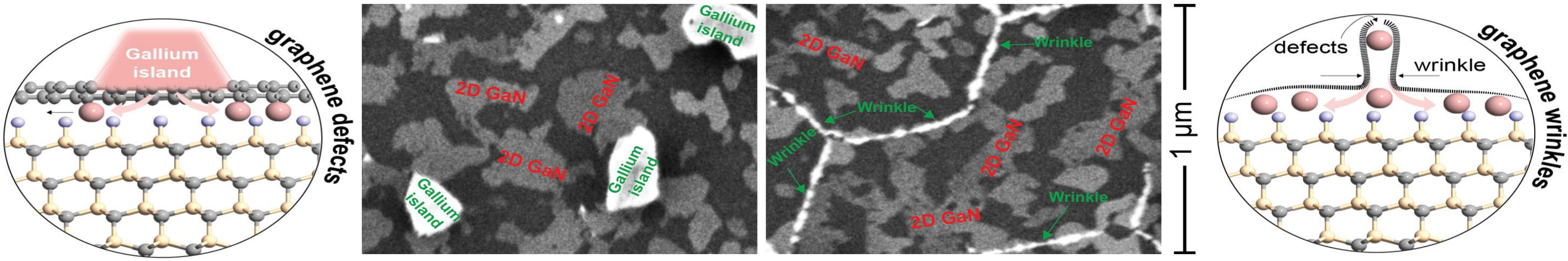
Ke Wang, PSU MCL



GaN Intercalation in Epi Graphene



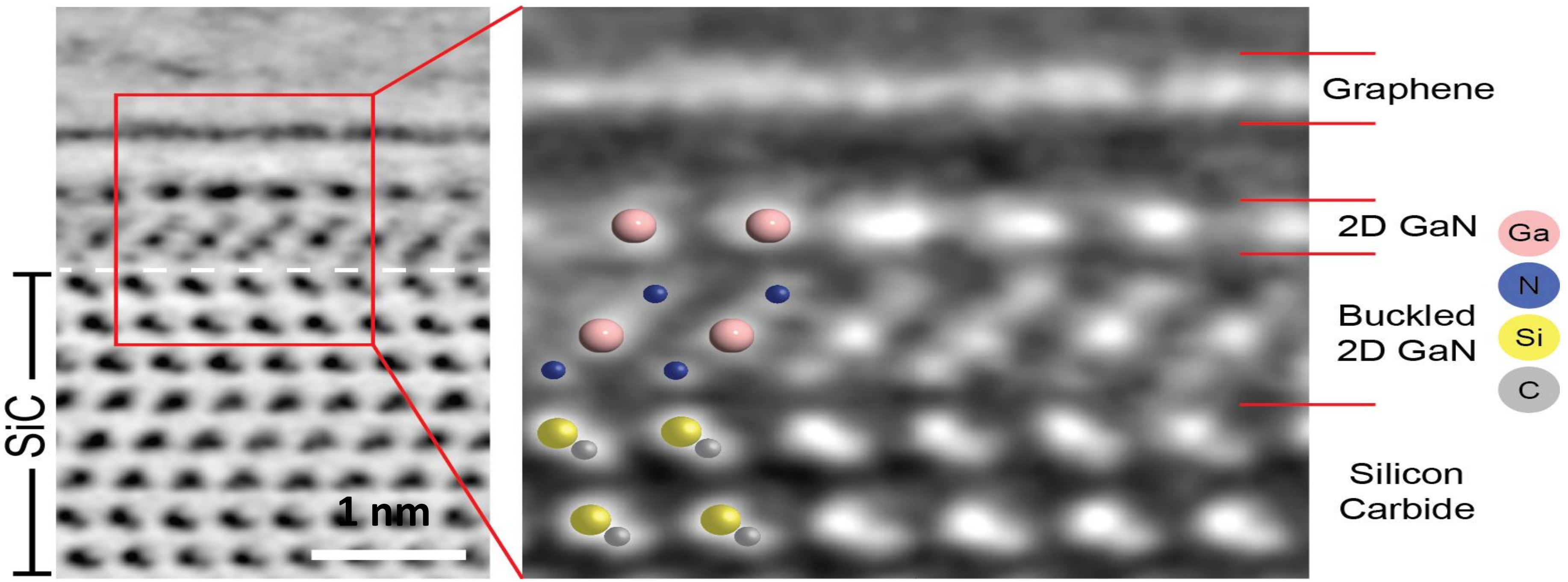
Pathways for Ga intercalation:

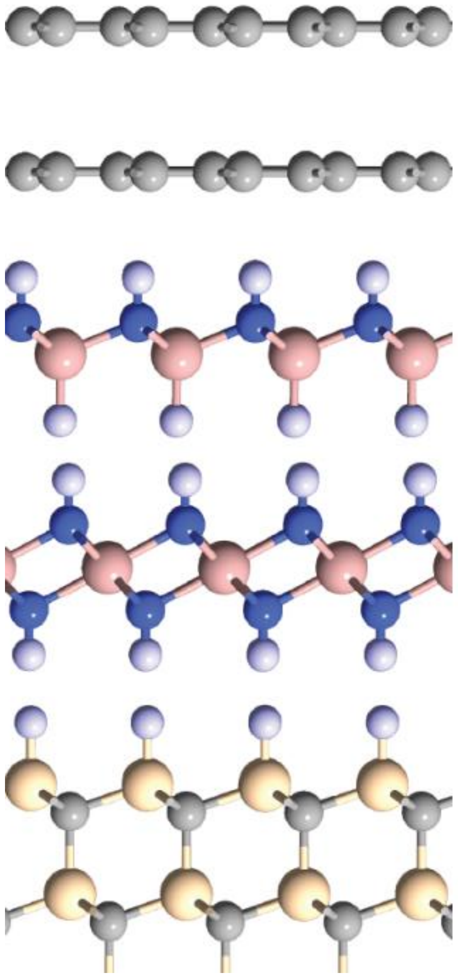


Atomic Structure of 2D GaN Layers

ABF STEM image near the $[11\bar{2}0]$ zone axis

Inverted image



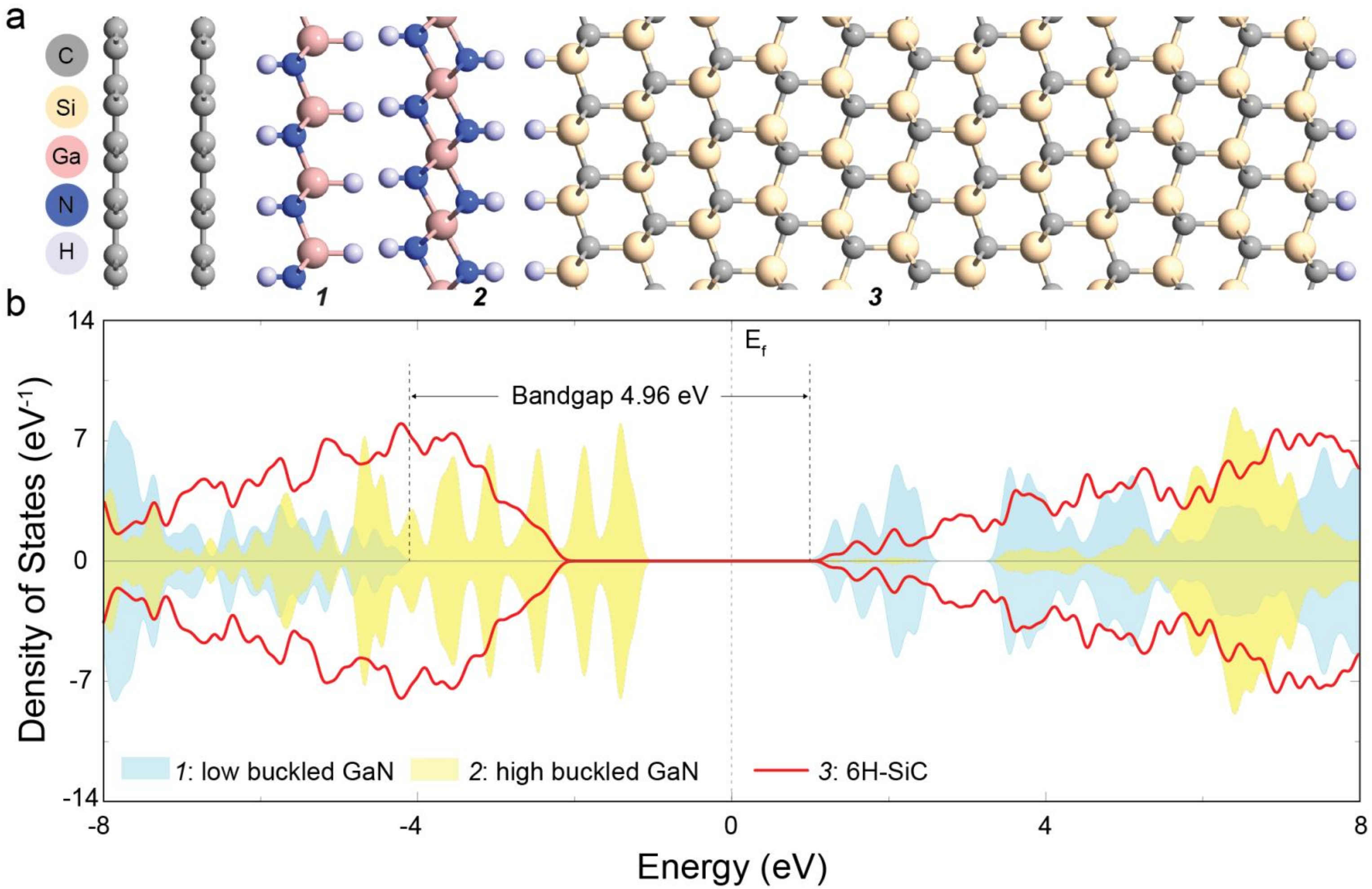


Two structurally different 2D layers of GaN at interface:

- Low buckled 2D GaN near graphene
- Highly buckled 2D GaN with nitrogen termination
- <u>Only</u> observed with graphene encapsulation

Ke Wang, PSU MCL

Electronic Structure of 2D GaN Layers



Predicted bandgap energies:

Low buckled GaN E_g=4.96 eV

High buckled GaN E_g=4.24 eV

Composite structure E_g=2.02 eV

Ram Krishna Ghosh and Suman Datta

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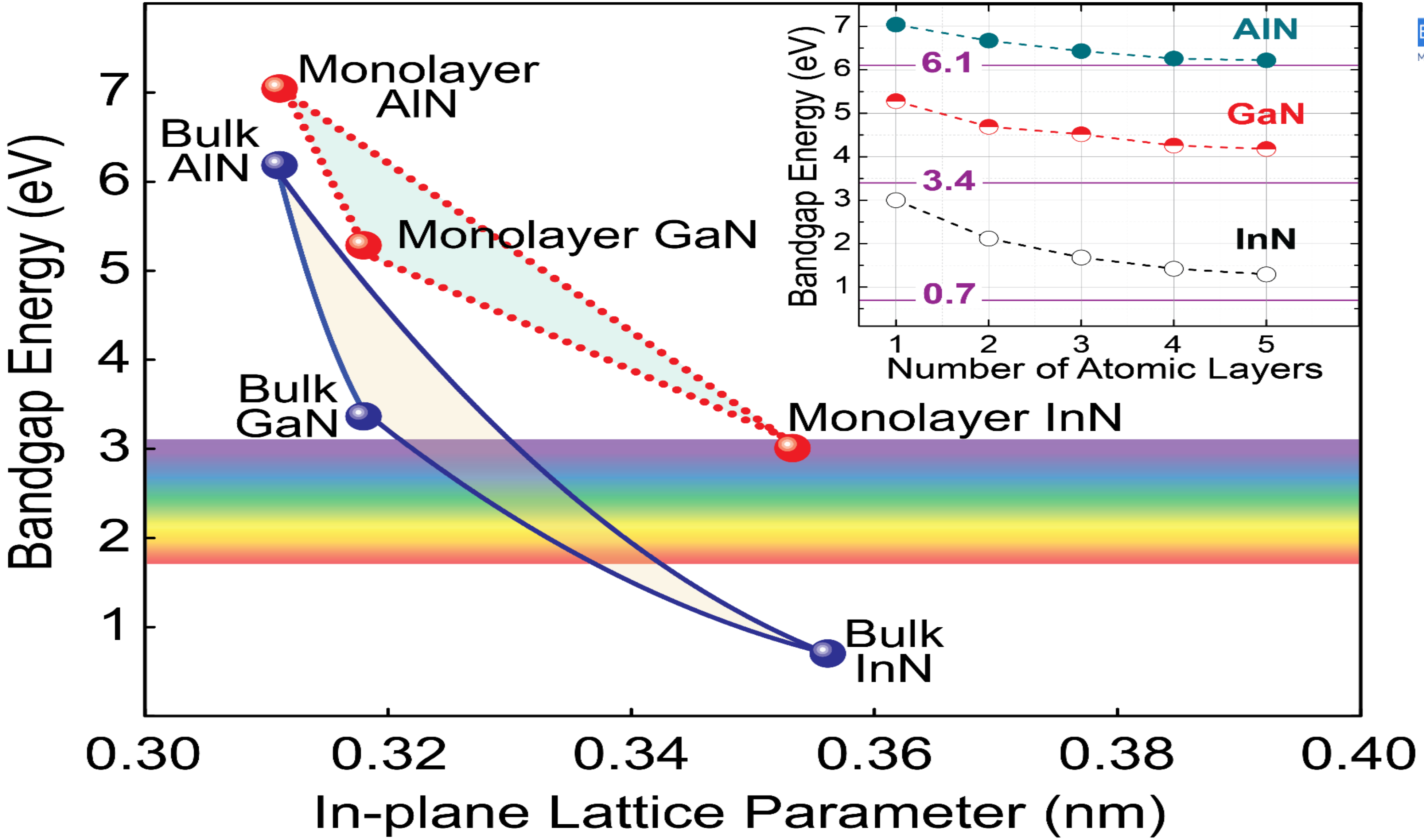

Summary

- MOCVD is a promising technique for TMDs and layered materials
- Graphene encapsulated MOCVD growth viable method to stabilize 2D GaN
- Future work directed at heterostructure growth, alloys & doping

Acknowledgements

PSU Collaborators
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Dr. Nasim Alem (MatSE)
Dr. Suman Datta (EE)
Dr. Ke Wang (MRI)
Dr. Tom Jackson (EE)

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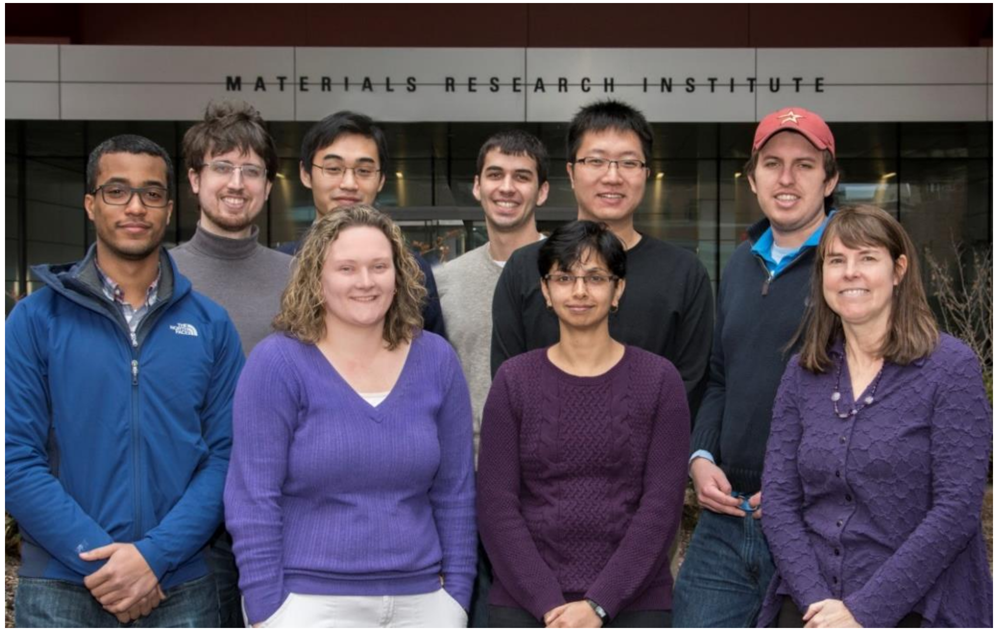
DOW



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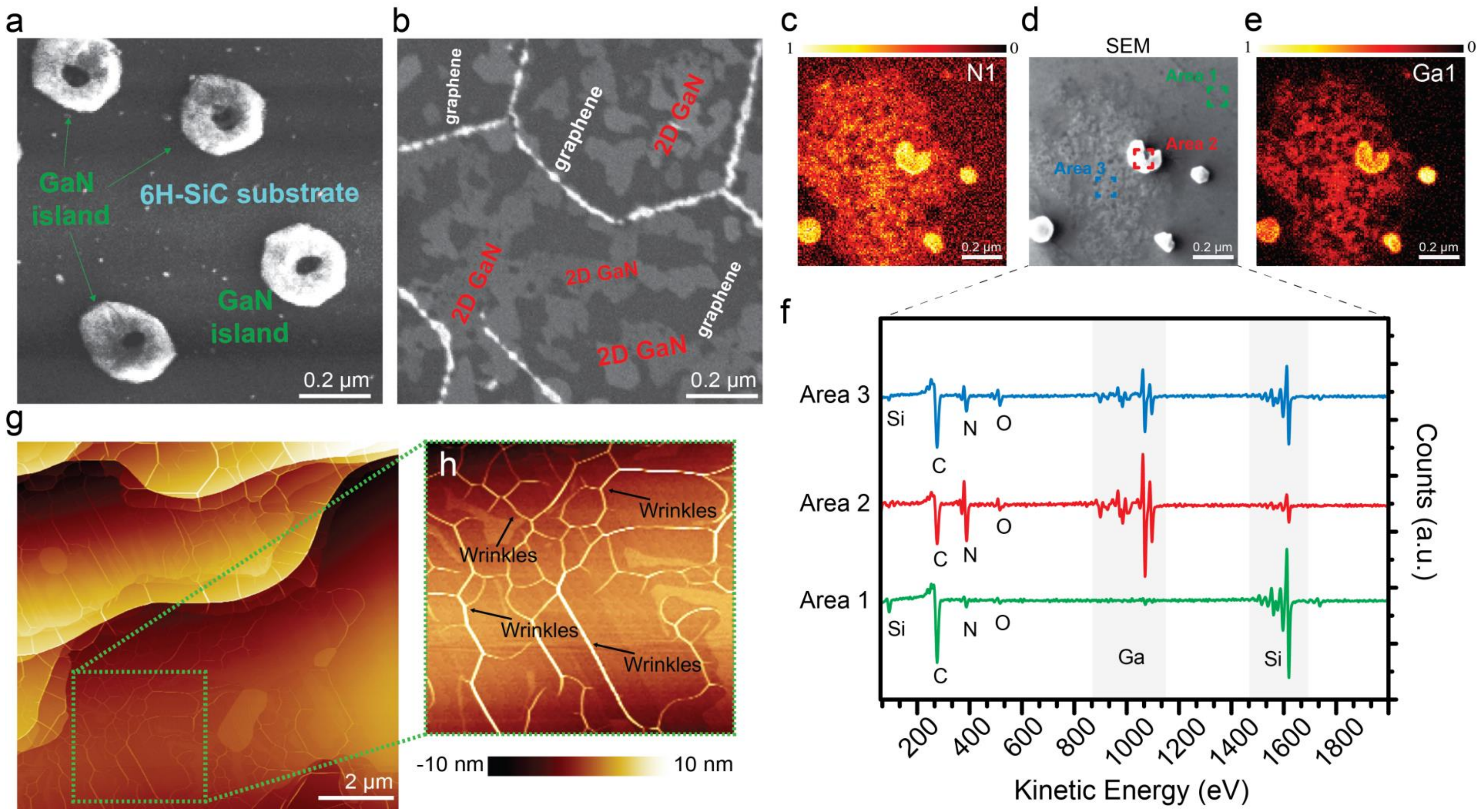
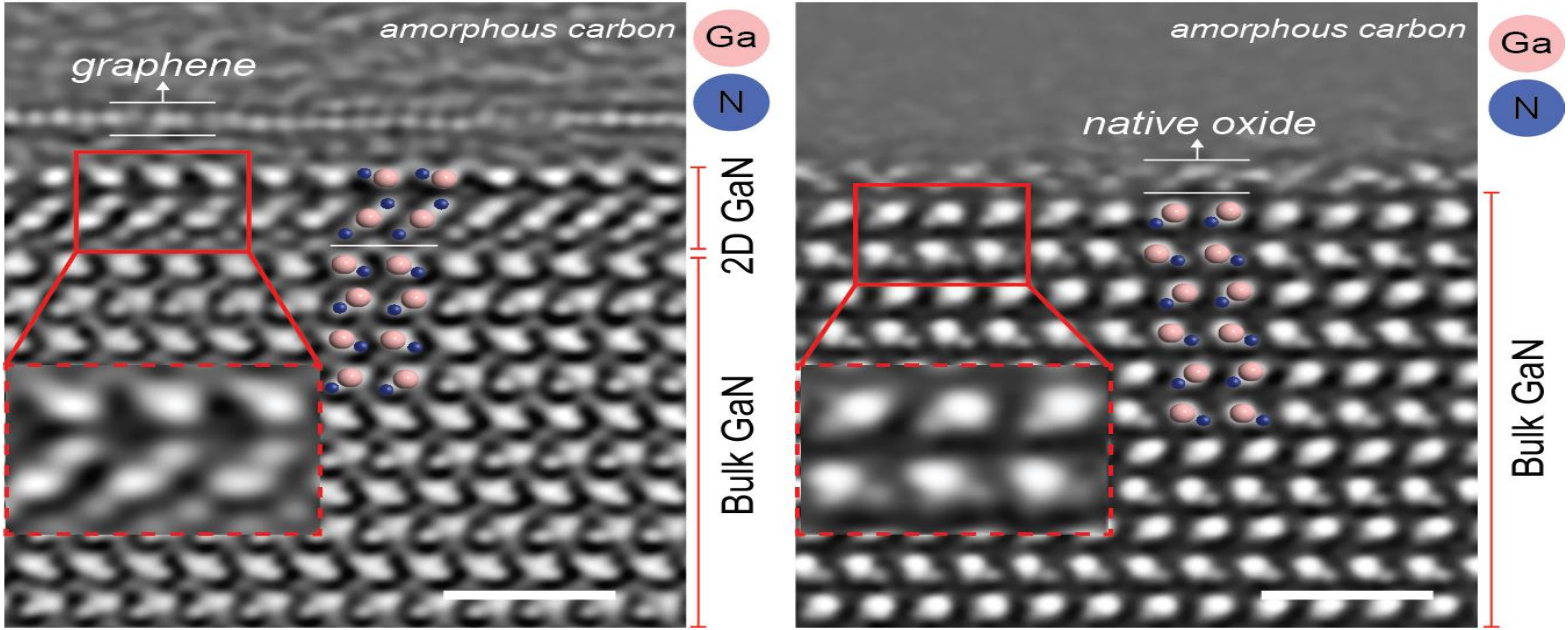
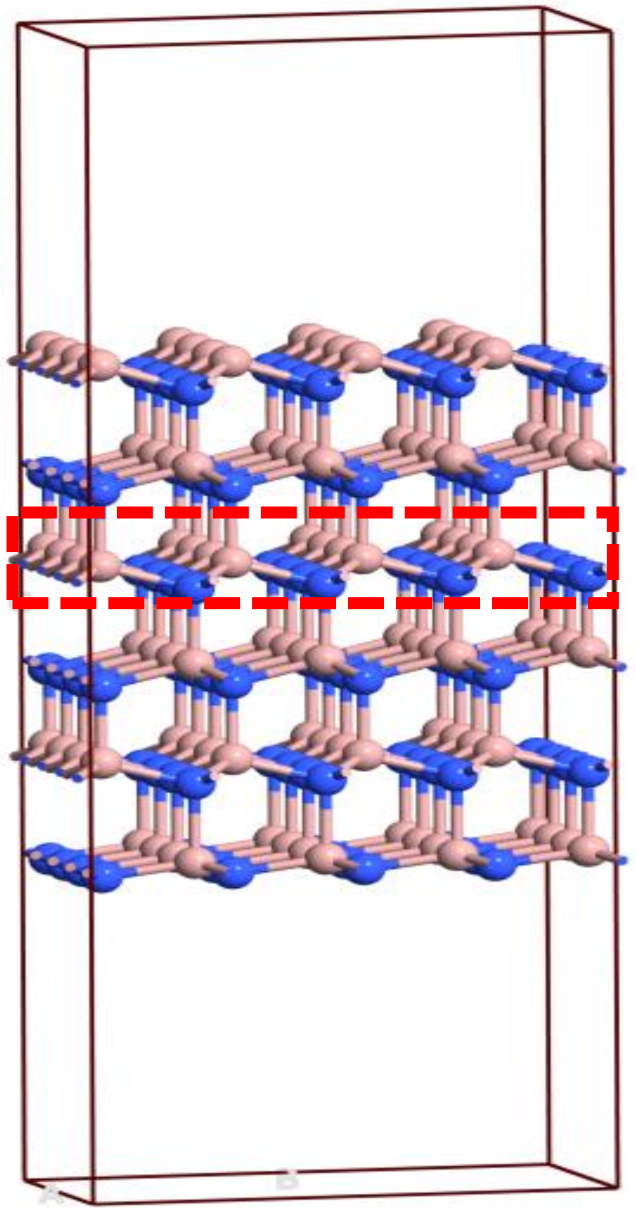
Tanushree Choudhury


a
GaN island
6H-SiC substrate
GaN island
0.2 μm
b
graphene
graphene
2D GaN
2D GaN
2D GaN
2D GaN
graphene
0.2 μm
c
N1
0.2 μm
d
SEM
Area 1
Area 2
Area 3
0.2 μm
e
Ga1
0.2 μm
f
Area 3
Area 2
Area 1
Si
C
N
O
Ga
Si
Counts (a.u.)
200
400
600
800
1000
1200
1400
1600
1800
Kinetic Energy (eV)
g
2 μm
h
Wrinkles
Wrinkles
Wrinkles
Wrinkles
-10 nm
10 nm


amorphous carbon
graphene
Ga
N
2D GaN
Bulk GaN
amorphous carbon
native oxide
Ga
N
Bulk GaN

Wurtzite Bulk Structure of GaN



Materials discovery with computation

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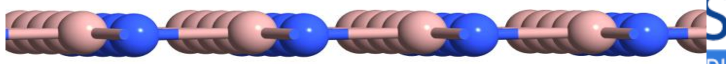
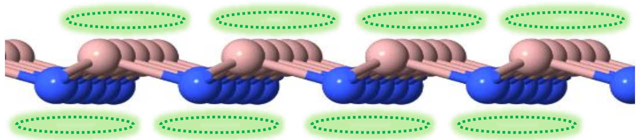
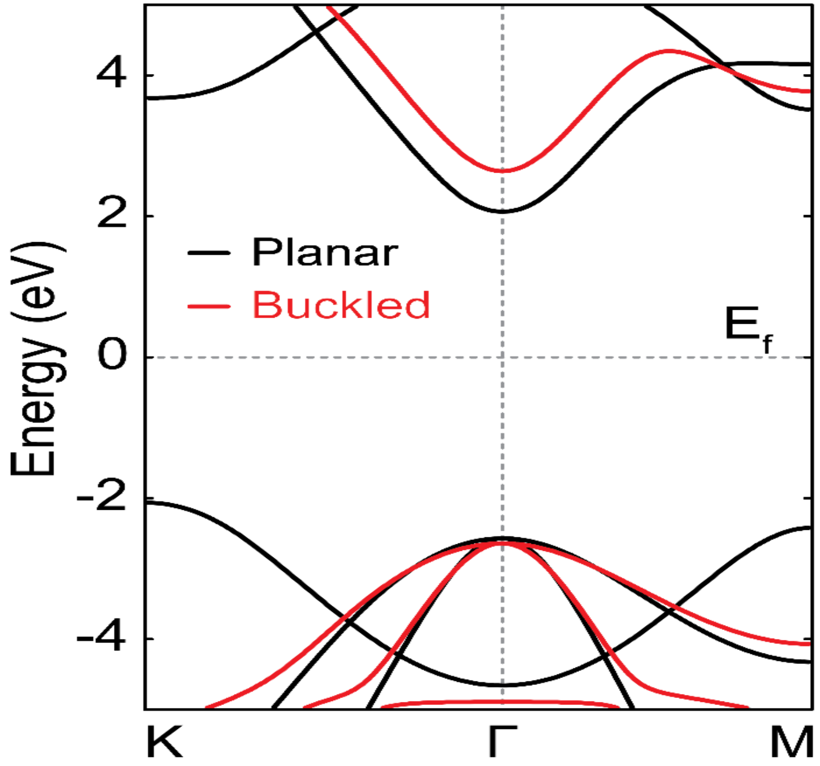
Indirect bandgap 4.12 eV

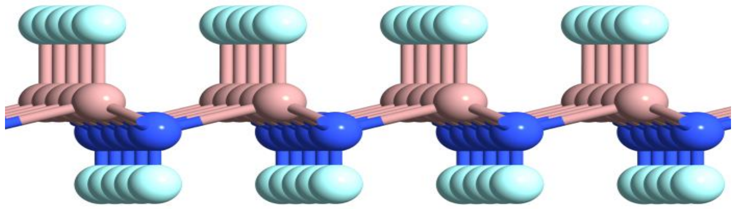




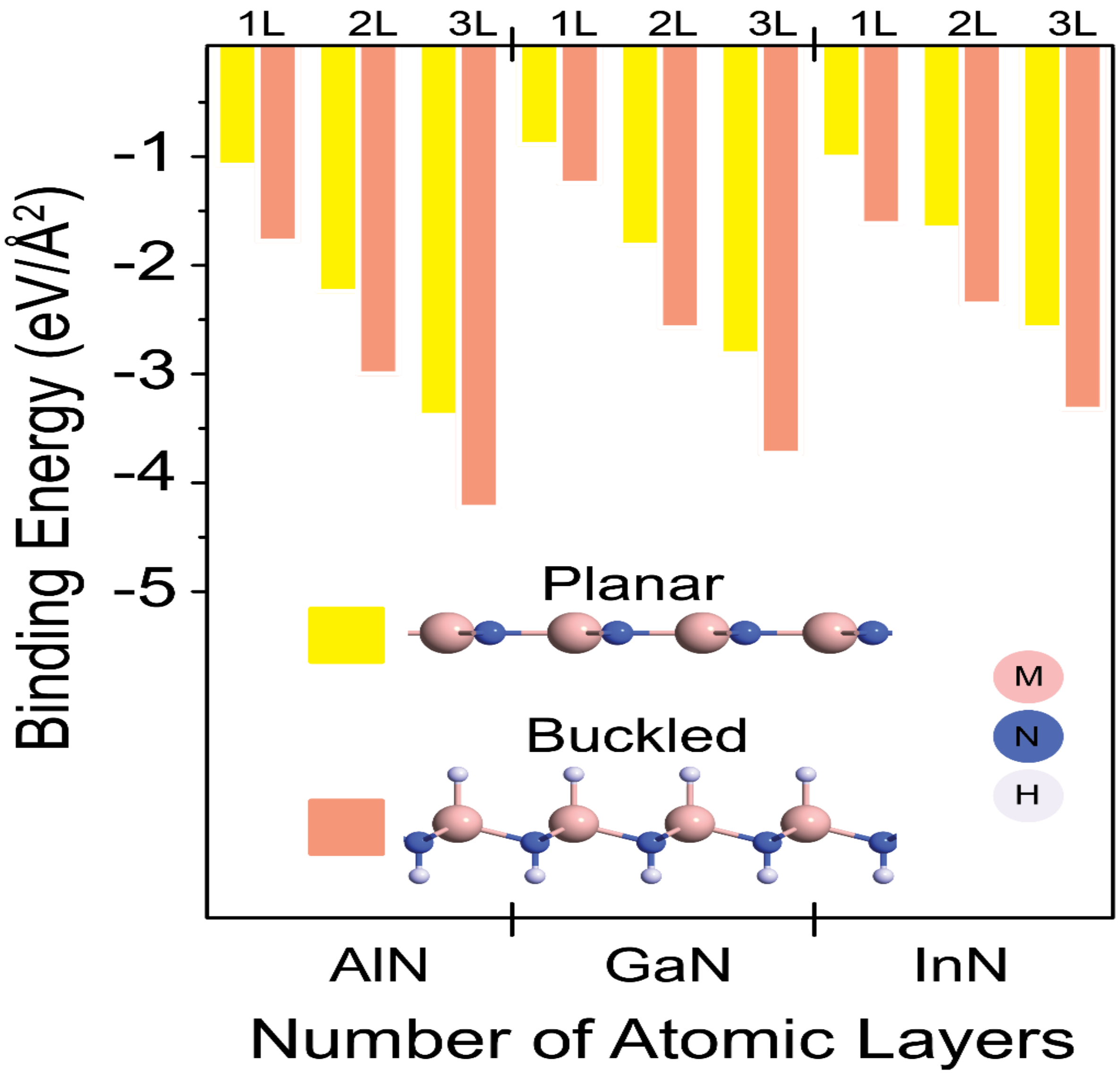
Stabilized Structure

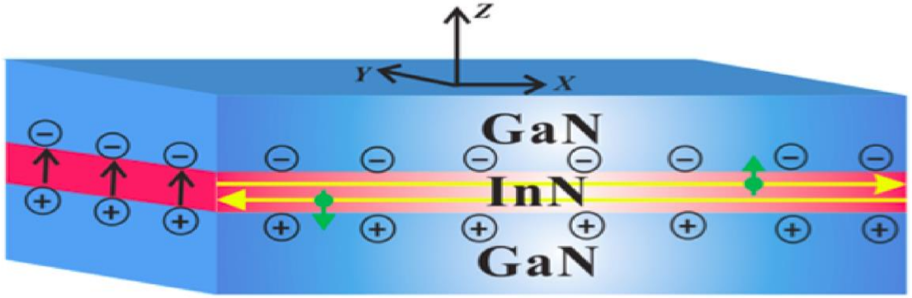


direct bandgap 5.28 eV



The Buckled Structure for 2D III-nitrides is More Stable!

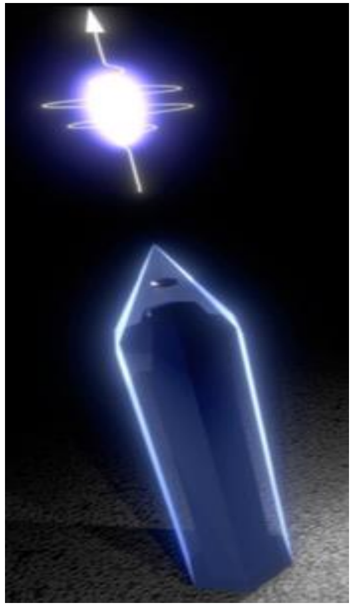




Polarization-induced Topological insulators for memory and quantum computing

Phys. Rev. Lett. **109,** 186803 (2012)

Exotic physics



Single-photon emitters for quantum optics and communication

Nano Lett. **14,** 982–986 (2014)

Nat. Mater. **5,** 887–892 (2006)