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PennState



RICE

ATOMIC

Center for Atomically Thin
Multifunctional Coatings



A National Science Foundation
Industry/University Cooperative Research Center



Two Universities



PennState



RICE



Integrated Solution

Director



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Co-Director



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Co-Director



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Site-Director



Jun Lou
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ATOMIC – Center Profile

- Approved by NSF in 2015; official launch in early 2016
- Currently in Phase I – moving toward Phase II (2020)

ATOMIC Center	
Total Faculty Funded	10
Number of Faculty in 2D & Coatings	30
Number of Students	6
Students Graduated	6
Total Lifetime Funding	\$2.1MM
Current Funding Level	\$640K
Number of Current Members	9
Full Membership Annual Dues	\$43,500
Associate Member Annual Dues	\$21,750

IAB Membership Roster

- Air Force Research Laboratory (AFRL)
- US Army Armament Research, Development and Engineering Center (ARDEC)
- Army Research Laboratory (ARL)
- Corning
- Evonik
- Honda Research Institute USA
- MilliporeSigma
- Morgan Advanced Materials
- Murata







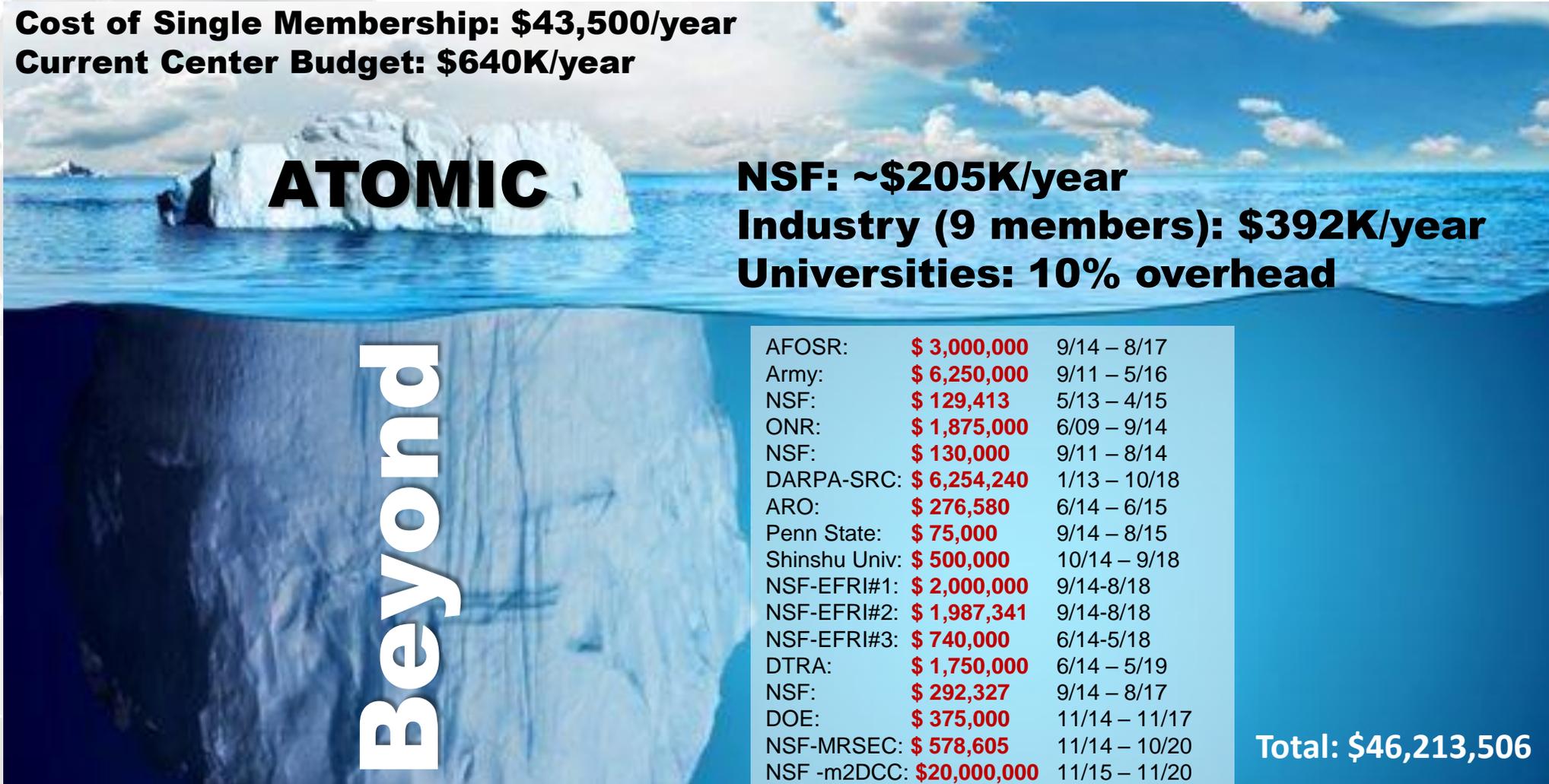




INNOVATOR IN ELECTRONICS

Beyond ATOMIC: Leveraging Expertise and Research Funding in 2D Materials to Accelerate Discovery and Transition

Cost of Single Membership: \$43,500/year
Current Center Budget: \$640K/year



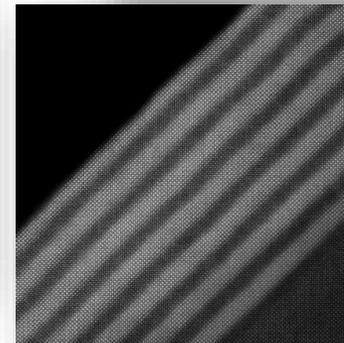
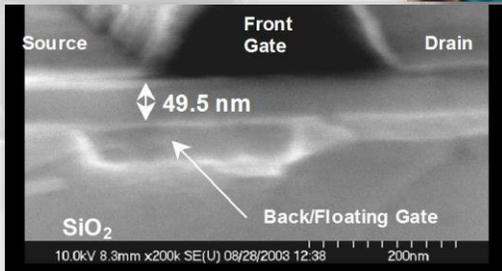
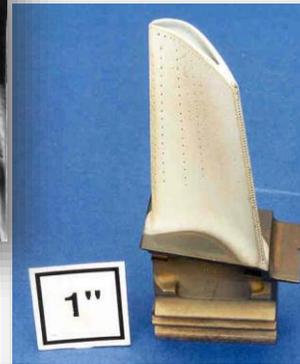
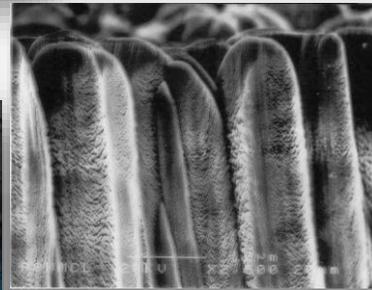
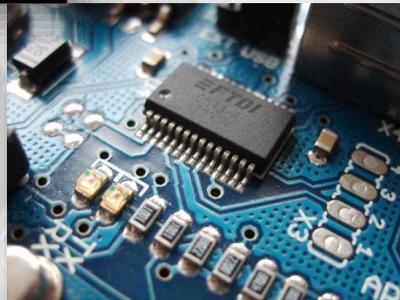
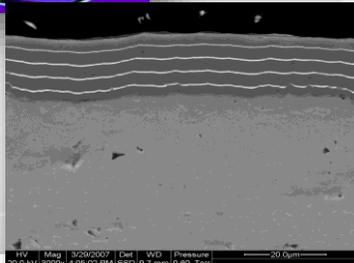
Leveraging your Membership Dollars

15:1

1150:1

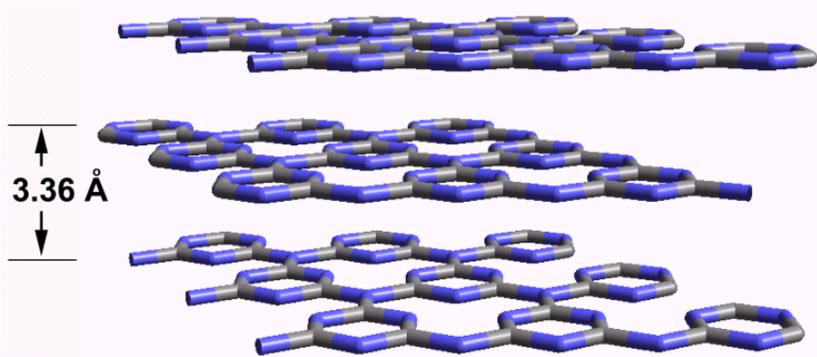
Total: \$46,213,506

Coatings Are Everywhere: What is next?

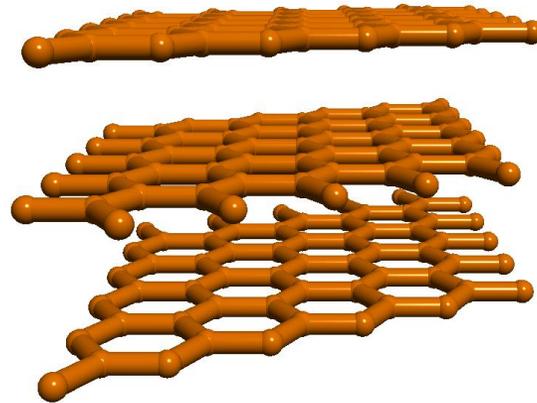


Perfect Layered Materials

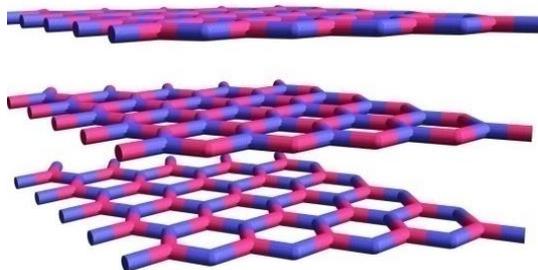
Carbon Nitride



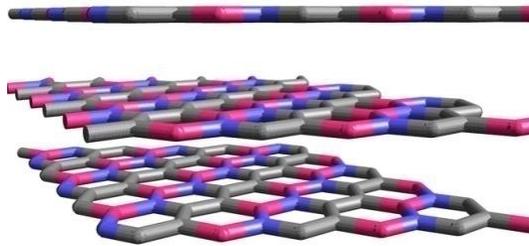
Graphite



Boron Nitride

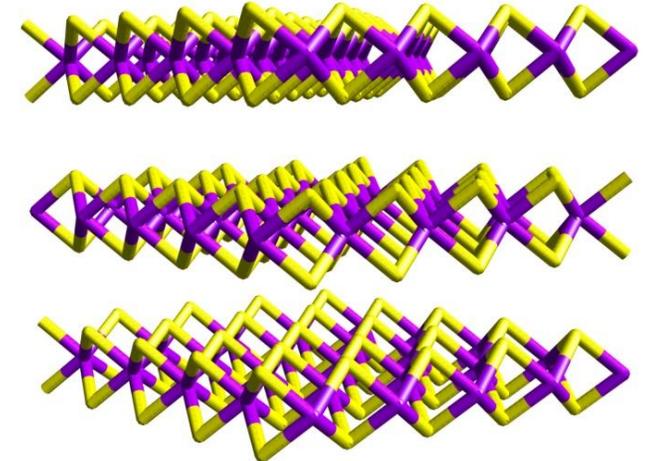


Boron Carbo-Nitride



Metal Chalcogenides

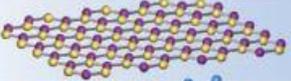
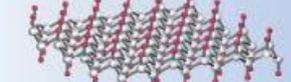
MoS₂
WS₂
NbS₂
TaS₂
VS₂
ReS₂
WSe₂
MoSe₂

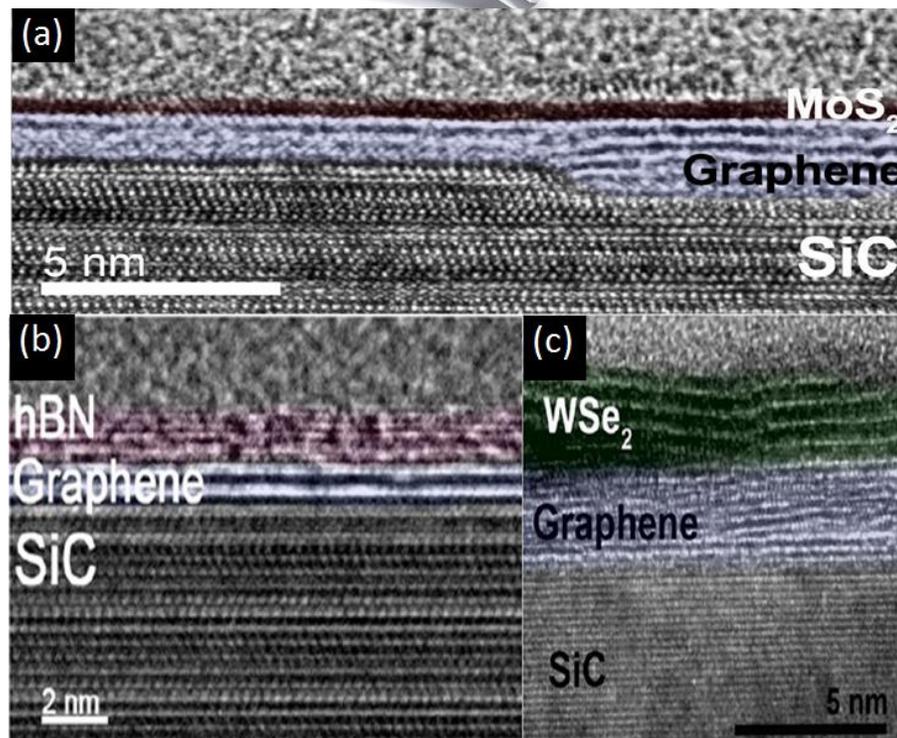
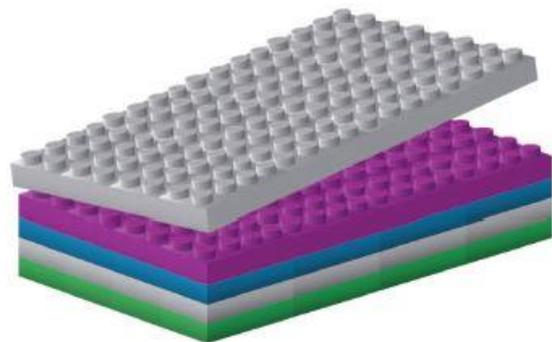


Chalcogenides

OTHERS VO₅, NiCl₂, MgB₂

Van der Waals Heterostructures

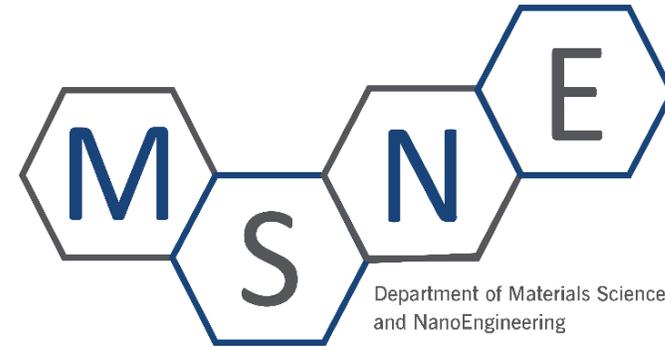
	Graphene	
	hBN	
	MoS ₂	
	WSe ₂	
	Fluorographene	



ATOMIC: One Family; Two Siblings



PennState
Materials Research
Institute



Leading the Way in 2D

- Penn State ranks #1 in Materials Engineering in the US*
- The Millennium Science Complex 2011 @ \$230MM
- World-class facilities including an NSF User-facility on 2D synthesis
- 30+ full time faculty and staff working on 2D Materials at PSU
- ATOMIC leverages expenditures in 2D research contracts totaling over \$46MM (1150:1)



Rice: Birthplace of Carbon Nanotechnology

1985 1990 1995 2000 2005 2010 2015 2020

1985:
Buckyball
Discovered
*Smalley¹, Curl¹
& Kroto²*

1991: Carbon
nanotubes
isolated
Sumio Iijima³

1996:
Nobel Prize
in Chemistry
*Smalley, Curl &
Kroto*

2004:
Graphene
isolated
*Geim⁴ &
Novoselov⁴*

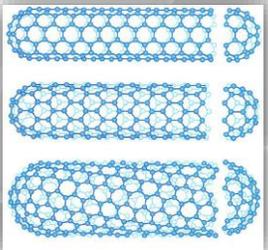
2010:
Nobel Prize
in Physics
*Geim &
Novoselov*

2013:
Materials Science
and Nano-
Engineering
department
launches
Rice

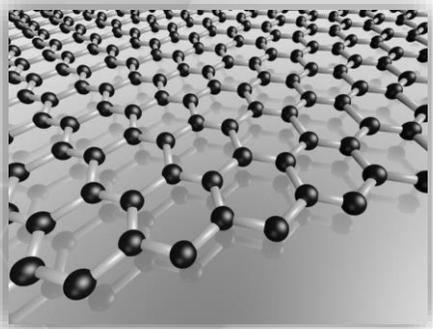
2016:
ATOMIC
launched
Rice & Penn
State

Rice work on carbon nanotubes starts with Smalley in early 1990s, and continues with many others, through to today. Rice's HiPCo (high-pressure carbon monoxide) process for growing nanotubes dominated for decades.

Late 1980s, early 1990s, Pulickel Ajayan¹ postdocs with Iijima



Shortly after Buckyball discovery, Smalley starts to theorize about carbon nanotubes

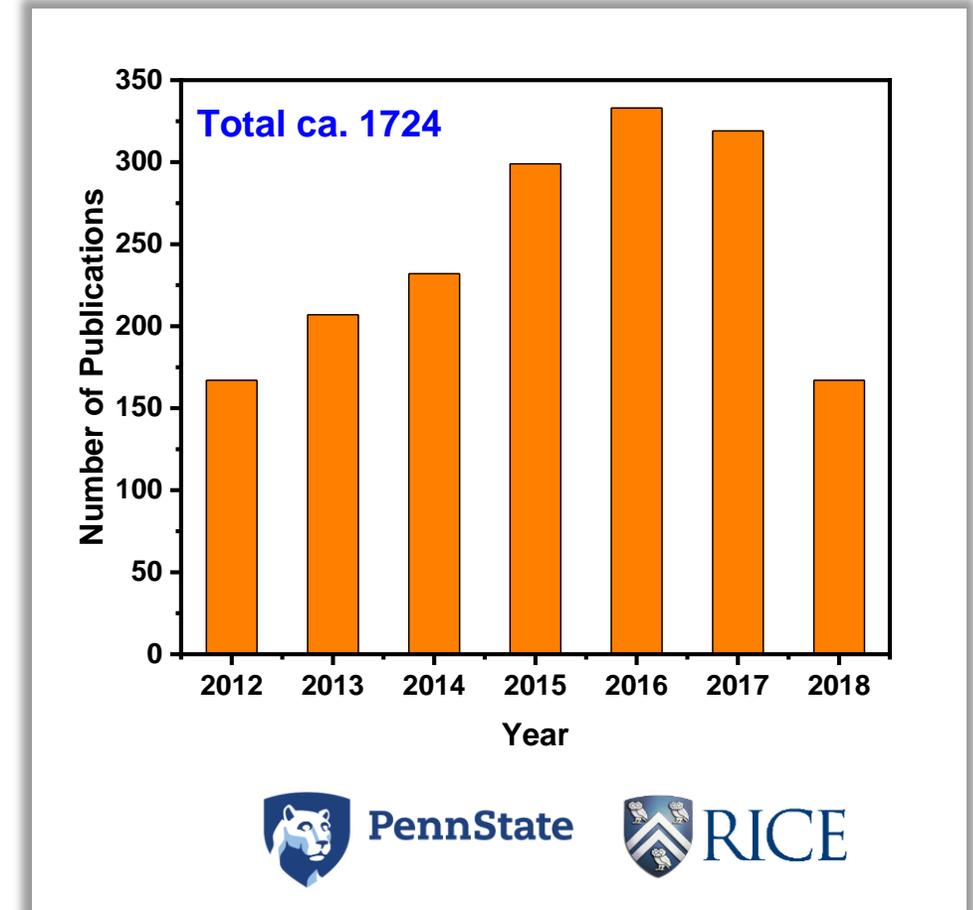
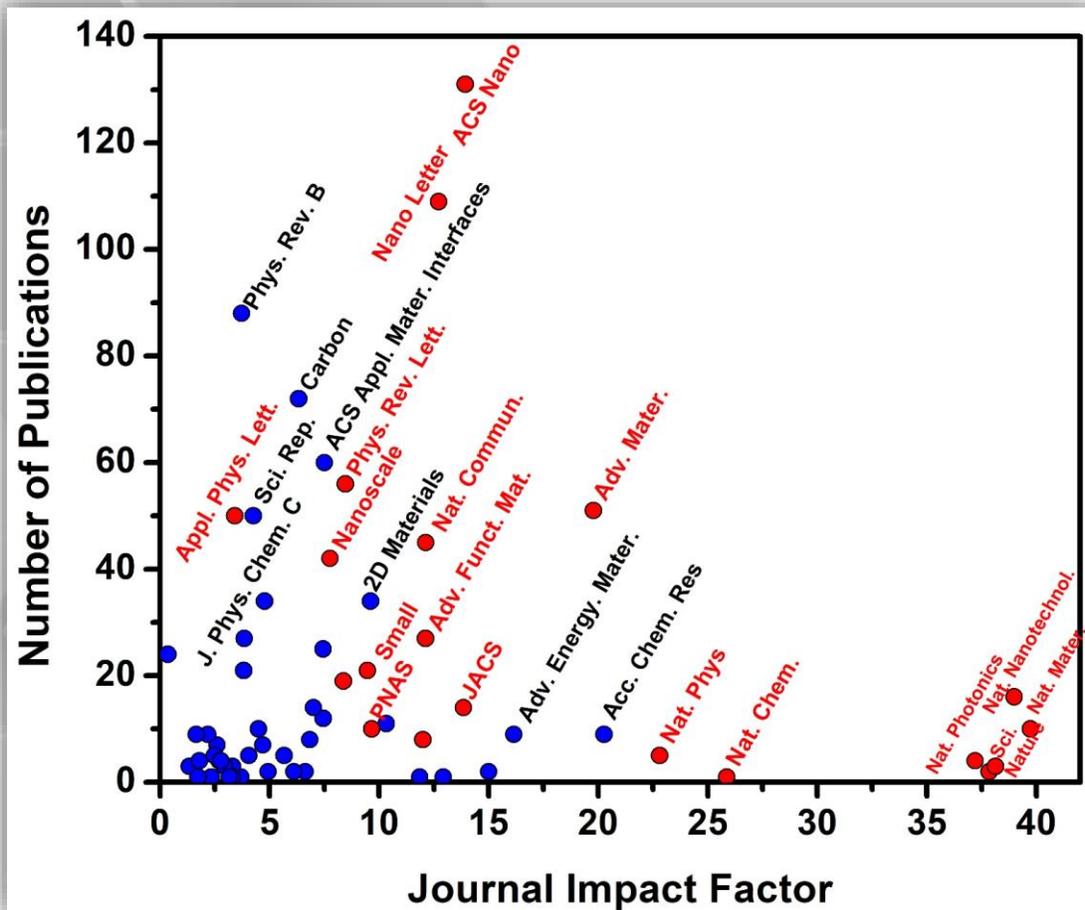


Rice work on graphene – mid-2000s to present

2D Materials research expands well beyond graphene and gains worldwide interest, with significant leadership from Penn State and Rice.

¹Rice University; ²University of Sussex (UK); ³National Institute of Advanced Industrial Science and Technology (Japan); ⁴University of Manchester (UK)

Rice and Penn State Dominate in Publications on 2D Materials



PennState



RICE

The Benefits of the I/UCRC Model

IUCRCs Provide Access To A Wide Variety Of Capabilities

- Not just one researcher or one group but multiple faculty across multiple departments and universities
- Pioneers in 2D Nanomaterials and Unique capabilities
- Very cost effective (access to 10x in funded research for a membership)

IUCRCs Focus On Solutions For Sponsor Defined Issues

The IP Guidelines Are Given By The NSF

- I/UCRC conducts pre-competitive research
- The research should be about defining a problem, not solving it

IUCRCs Provide Excellent Networking Opportunities

- Suppliers, competitors, customers
- Personal relationship building: learn about each other's needs. Monthly mentoring calls.

IUCRCs Provide Excellent Recruiting Opportunities

- Interact with students twice a year and follow their technical, communication, and interpersonal skill development

IAB: Selecting/Prioritizing Topics

Topics Suggested by Members During Visits With Directors/Faculty

Throughout Year

Call for Proposals to Faculty based on Topics of Interest

Prior to IAB Meeting

Proposals Voted on by IAB

Full Members = 6 votes
Assoc. Member = 3 votes

Funded Proposal
1

Funded Proposal
2

Funded Proposal
.....X

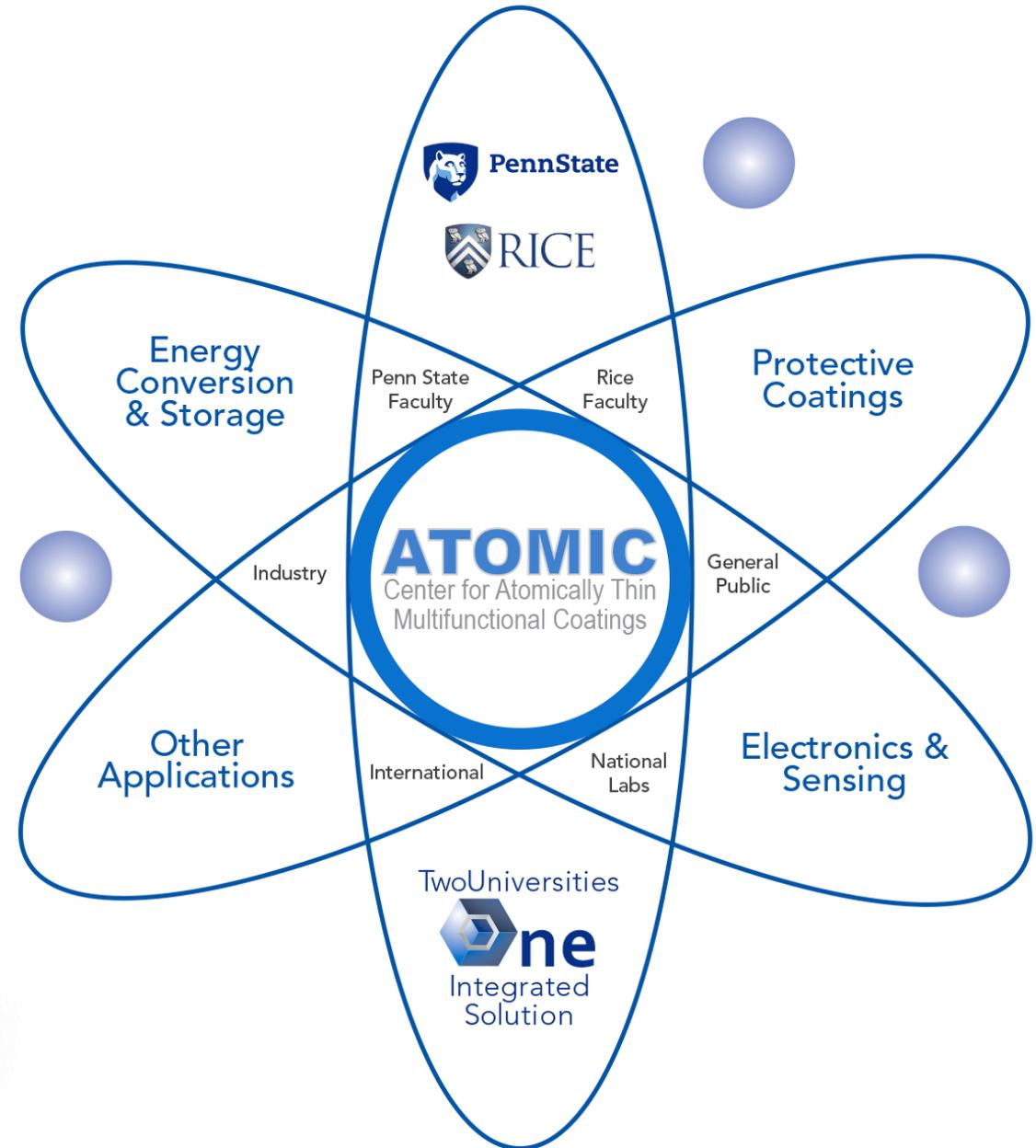
of Funded Proposals
Depends on # of
Members and Funding

Seed Project

Seeds Future Proposals



ATOMIC Topics



Atomic Layers For Multifunctional Protective Coating At High Temperature, High Pressure Extreme Conditions

Shuai Jia, Steven Schara(students); Jing Zhang (Postdoc); Jun Lou (PI)

Project Overview

- New coating that can work at high temperature and pressure conditions is highly desired for many industry applications, such as oil drilling, chemical reaction reactor.
- This project aims to synthesis directly high quality, ultra-dense and large-area hexagon boron nitride (h-BN) coating on various industry components with different compositions and shapes, such as stainless steel plates, and tungsten carbides balls.
- We will utilize them as anti-abrasion, anti-erosion and anti-corrosion coating at high temperature (200-600 °C) and high pressure (>10 MPa) extreme conditions, and evaluate their performance and cost as compared with current technologies for anti-abrasion and anti-corrosion at extreme conditions.
- Project start date/proposed length of project: May 2018; 24 months

Major Findings

- In our previous project, we developed method to grow continuous h-BN film on stainless steel substrate by CVD method. In this continuation project, we extended h-BN growth method to carbon steel substrate and even curved substrate, like tube. The high and sharp Raman peak demonstrate its quality is as high as that on stainless steel.

Figure1. CVD grown h-BN on stainless steel. (a-b) SEM images, inset is optical images before and after h-BN growth. (c) cross-section images of h-BN coated stainless steel. (d-f) XRD, Raman, and XPS depth profile of h-BN on stainless steel.

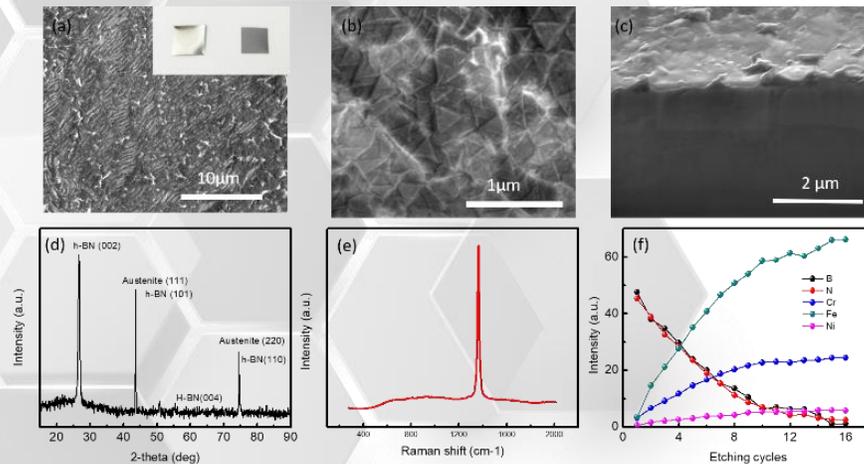
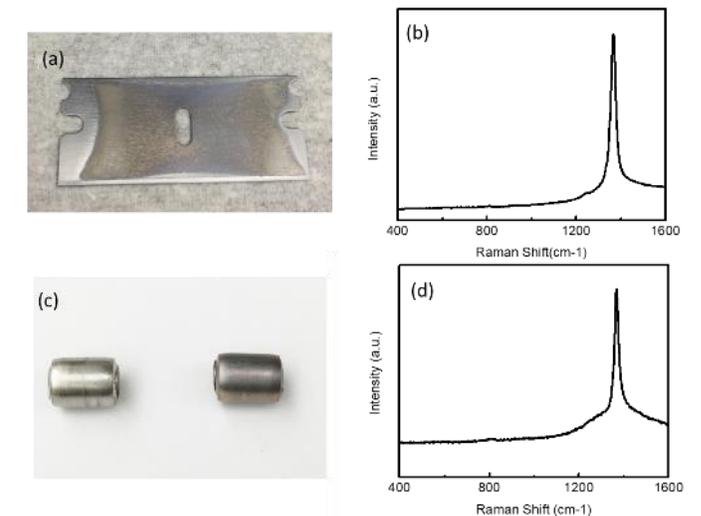


Figure2. CVD grown h-BN on carbon steel and stainless steel tube. (a-b) optical images and Raman of h-BN grown on carbon steel. (c-d) optical images and Raman of h-BN grown on stainless steel tube.



Atomic Layers For Multifunctional Protective Coating At High Temperature, High Pressure Extreme Conditions – *What We Did*

We functionalized h-BN powder with different functional groups by ball milling method (NaOH for –OH, Urea for –NH₂, Oxalic acid for –COOH). After functionalization, h-BN could form stable suspension. No precipitation is observed for functionalized h-BN after several days. The FTIR and XPS spectra both demonstrated some functional group is successfully anchored onto h-BN sheets.

Standard salt spray test was used to characterize anti-corrosion performance of h-BN coating for carbon steel. Lots of corrosion dust (dark orange particles) appeared on bare carbon steel just for 1 day testing. While, no obvious surface changes is observed for both h-BN/PVDF and CVD h-BN coated carbon steel. This is the strong evidence for the excellent anti-corrosion performance of h-BN films.

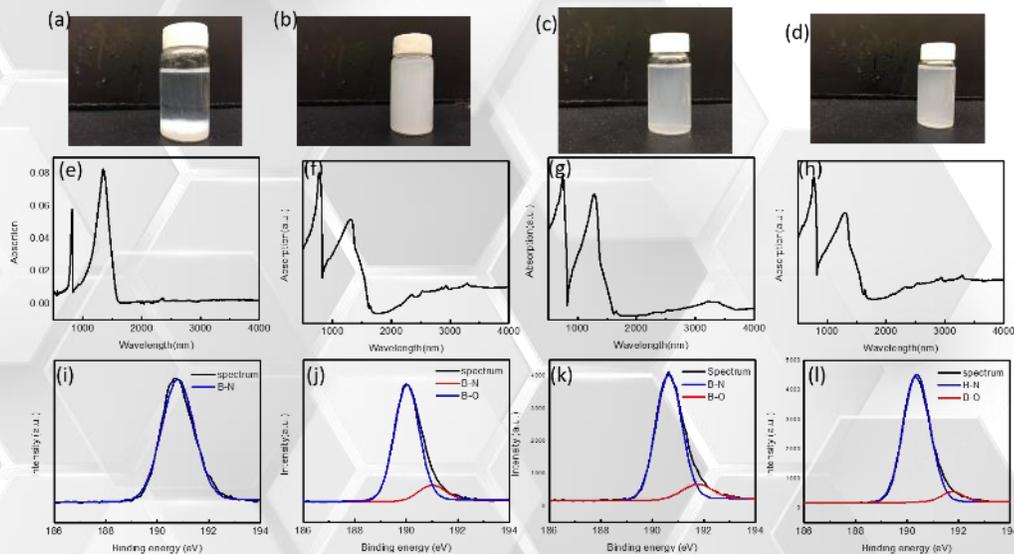


Figure 3. h-BN functionalization with different functional groups. (a-d) suspension of h-BN, h-BN-OH, h-BN-NH₂, h-BN-COOH. (e-h) FTIR spectra of h-BN, h-BN-OH, h-BN-NH₂, h-BN-COOH. (i-l) XPS of B element of h-BN, h-BN-OH, h-BN-NH₂, h-BN-COOH.

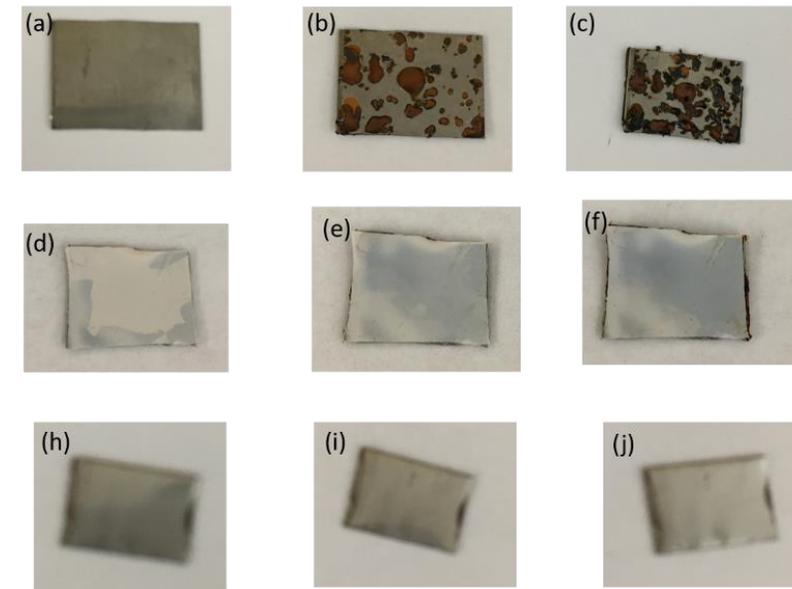


Figure 4. Optical images of salt-spray tested samples. (a-c) bare carbon steel images for 0,1,2 days testing. (d-f) h-BN/PVDF coated carbon steel images for 0,1,2 days testing. (h-i) CVD grown h-BN on carbon steel images for 0,1,2 days testing.

Low Temperature/Low Cost Deposition of 2D Materials On Metals And Conducting Glass For Protective And Energy Conversion Applications (Topic: Scalable Routes)

Yu Lei, Fu Zhang, Kazunori Fujisawa, Néstor Perea-López, Ana Laura Elias PI: Mauricio Terrones

Project Overview

Opportunity / need being addressed

- An economical and scalable electrodeposition route to synthesize MoS₂ and graphene few-layer coatings on ITO, stainless steel, and glassy carbon.
- Design and synthesize multifunctional sandwich hetero-structures using MoS₂, and graphene.
- Tuning the catalytic, optical, mechanical and electronic properties of the electrodeposited MoS₂ film via hetero-atom, including V and N.

Value proposition – why sponsor is interested

- Low cost, transparent layered durable coatings on metallic surfaces with applications in wear resistance, anti-corrosion, anti-oxidation, catalytic, energy conversion, etc.

Proposed project concept / research

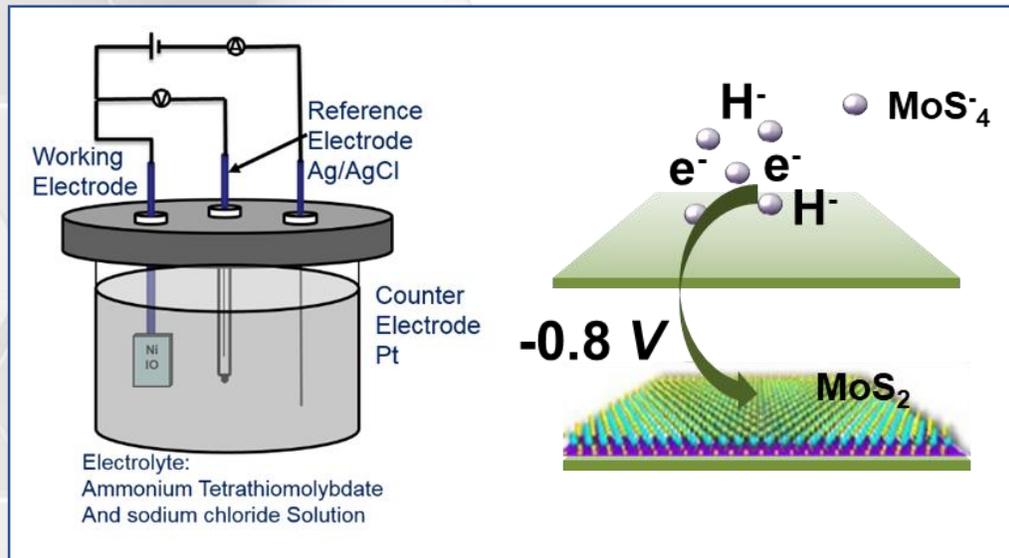
- Low cost multifunctional coatings on conducting substrates based on MoS₂, and graphene by electrodeposition.
- Heterolayers design among different 2D materials to achieve multifunctionality.
- Hetero-atom doping in electrodeposited MoS₂ at low temperature for multifunctionality.

Low Temperature/Low Cost Deposition of 2D Materials On Metals And Conducting Glass For Protective And Energy Conversion Applications (Topic: Scalable Routes)

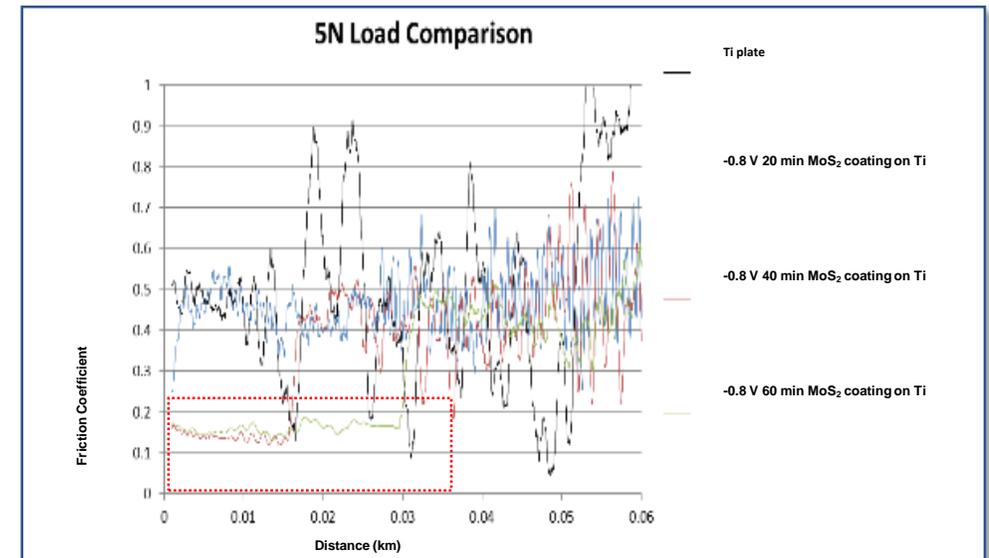
Yu Lei, Fu Zhang, Kazunori Fujisawa, Néstor Perea-López, Ana Laura Elias **PI: Mauricio Terrones**

Major Findings

1. Electrodeposition of MoS₂ coatings on conducting substrates.



2. Lower friction coefficient (0.15) in electrodeposition of MoS₂ coatings.



3. Heterolayer rGO/MoS₂ can be synthesized by layer-by-layer electrodeposition to be used as a photoelectrochemical catalyst for hydrogen evolution reaction

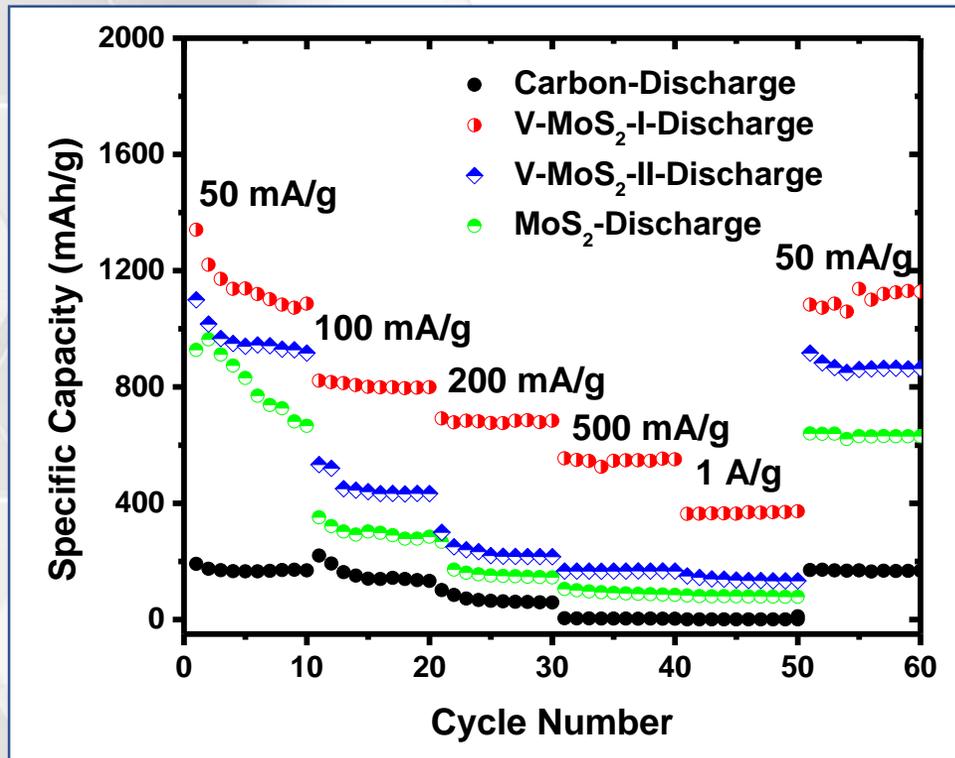
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Major Findings

4. V doped MoS₂ synthesized at 800 C and 400 C for high capacitance Li-ion anode, and HER catalyst.

5. N doped MoS₂ synthesized at different temperature 650, 550, and 450 to improve anti-wear performance. The coating also showed HER active as a multifunctionality.



Funded Projects (May 2018)

1. 2D/3D Hybrid Semiconductors for Electronics and Sensing
Thrust: Electronics & Sensing
2. Benchmarking Fenton Reactions with ATOMIC for Sensing and Catalysis
Thrust: Electronics & Sensing
3. Benchmarking Electronic, Sensing and Statistical Properties of 2D Films
Thrust: Electronics & Sensing
4. Low-Temperature Deposition of 2D Hetero-Materials on Conducting Substrates for Protective, Energy Conversion, And Sensing Applications
Thrusts: Protective Coatings, Energy Conversion, and Sensing
5. Atomic Layers for Multifunctional Protective Coating at High Temperature And Extreme Conditions
Thrust: Protective Coatings
6. Integrated Sensor-Power Coatings Utilizing Two-Dimensional Materials
Thrusts: Sensing and Energy Storage

Completed Projects (Jan. 2016 – May 2018)

1. Electronically Active 2D/3D Heterostructures
2. Low Temperature Chemical Vapor Deposition of 2D Layers for Energy, Protection, and Multifunctional ATOMIC
3. Low Temperature and Low Cost Deposition of 2D Materials on Metals and Conducting Glass for Protective and Energy Conversion Applications
4. Atomic Layers for Anti-Corrosion Coatings
5. Development of Atomically Thin Materials Based Coatings for Electrochemical Energy Storage
6. 2D Materials Defects: Characterization and Impact on Performance and Reliability
7. Reliability and Multifunctionality for Next Generation Coatings

Completed Seed Projects (March 2017)

Seed Project 1. "Modeling Growth Morphology of h-BN Using a Multiscale Approach"

Seed Project 2. "Boron Nitride Coatings for Low Friction and Wear"

Seed Project 3. "Design of 2D-Material-Based Multifunctional Hierarchical Structure"

ATOMIC Member Testimonials



**Dr. Phil Armstrong, Lead
Carbon Science Centre of Excellence
Morgan Advanced Materials**

- What does Morgan gain from ATOMIC?
- Describe your experience as an IAB member and as Co-Chair

Millipore Sigma

Dr. Shashi Jasty, Director
Global Technology Development
MilliporeSigma

- Describe how the IAB drives the direction of ATOMIC

How Can You Get Involved?

Industry Advisory Board Meeting

May 6-7, 2019

State College, PA

Visitors welcome!

- Updates on all current projects
- Opportunity to meet members, see how center works
- Poster session – see emerging topics and talent
- *Non-members are required to sign an NDA

Questions?

Interested in university-industry partnerships?

Sign up for information about UIDP news, webinars, projects, and more at uidp.org/newsletter-signup.



Strengthening
University-Industry
Partnerships

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