



# Exploring 2D materials in emerging solar cells

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Energy Materials Research Lab (EMRL)



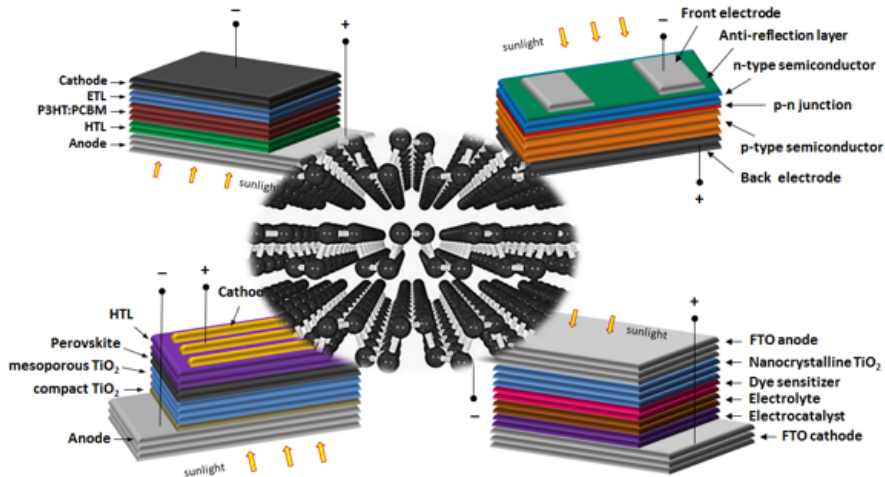
**QUEENSLAND MICRO- AND  
NANOTECHNOLOGY CENTRE**



**SCHOOL OF ENVIRONMENT  
AND SCIENCE**

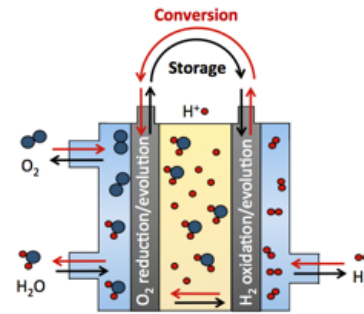
# Research Interest in "Nanomaterials for Energy"

## Solar Cells

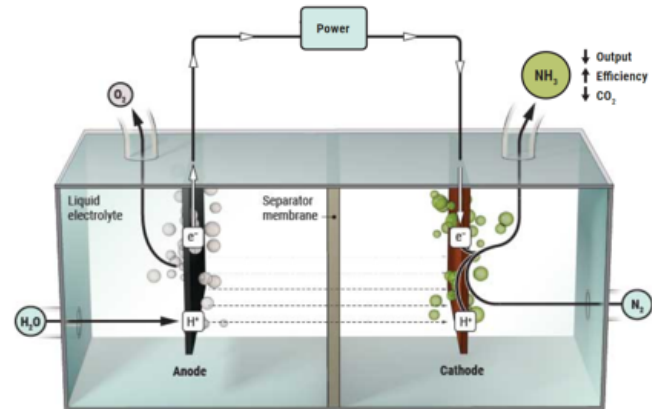


- *Adv. Mater*, **2020**, 32, 2000631.
- *Adv. Energy Mater*, **2020**, 10, 1902253.
- *Angew. Chem. Int. Ed*, **2019**, 58, 5202.
- *Angew. Chem. Int. Ed*, **2018**, 57, 2644.
- *Adv. Energy Mater*, **2018**, 8, 1701832.
- *Adv. Sci*, **2017**, 4, 1600504.
- *Adv. Mater*, **2016**, 28, 8586.

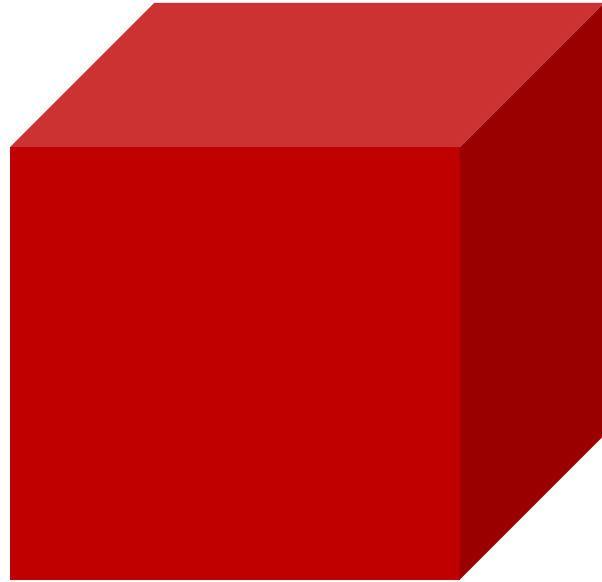
## Catalysis



- *Adv. Funct. Mater*, **2022**, 32, 1207280.
- *Small*, **2021**, 17, 2102218.
- *Angew. Chem. Int. Ed*, **2020**, 60, 2541
- *Adv. Mater*, **2019**, 31, 1900546.
- *J. Mater. Chem. A*, **2020**, 8, 4735.
- *J. Mater. Chem. A*, **2020**, 8, 15875.



# Sun Power – Solar Tech



Solar Energy on Earth's  
atmosphere  
(10,000 times higher than GED)



Global Electricity  
Demand (GED)  
(>25,000 terawatt hours)



Current PV  
installations  
(~50 times lower than  
GED)

# Solar Cells in the Market



## Silicon – Solar Cells

Performance:

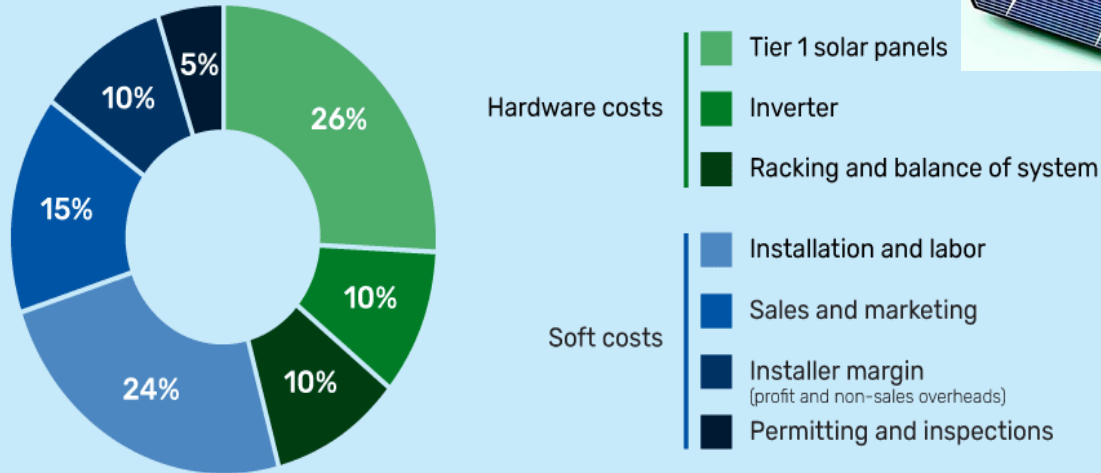
High efficiency

Cost:

**High**

# PV market

## Solar installation cost breakdown

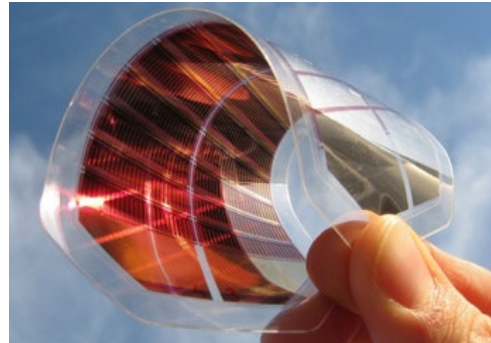
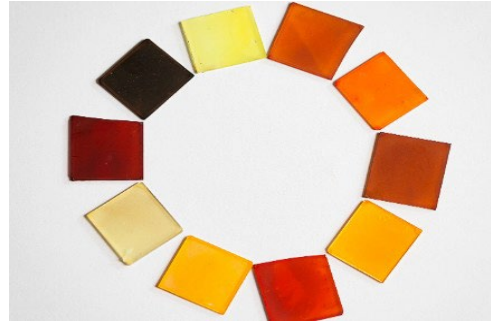


## Potential solutions:

- BIPVs (other applications such as windows)
- Increase PV performances
- Constructing tandem solar panels (highly performance)
- Lowering the panel cost significantly
- Simplifying panel architecture

# Emerging Solar Cells

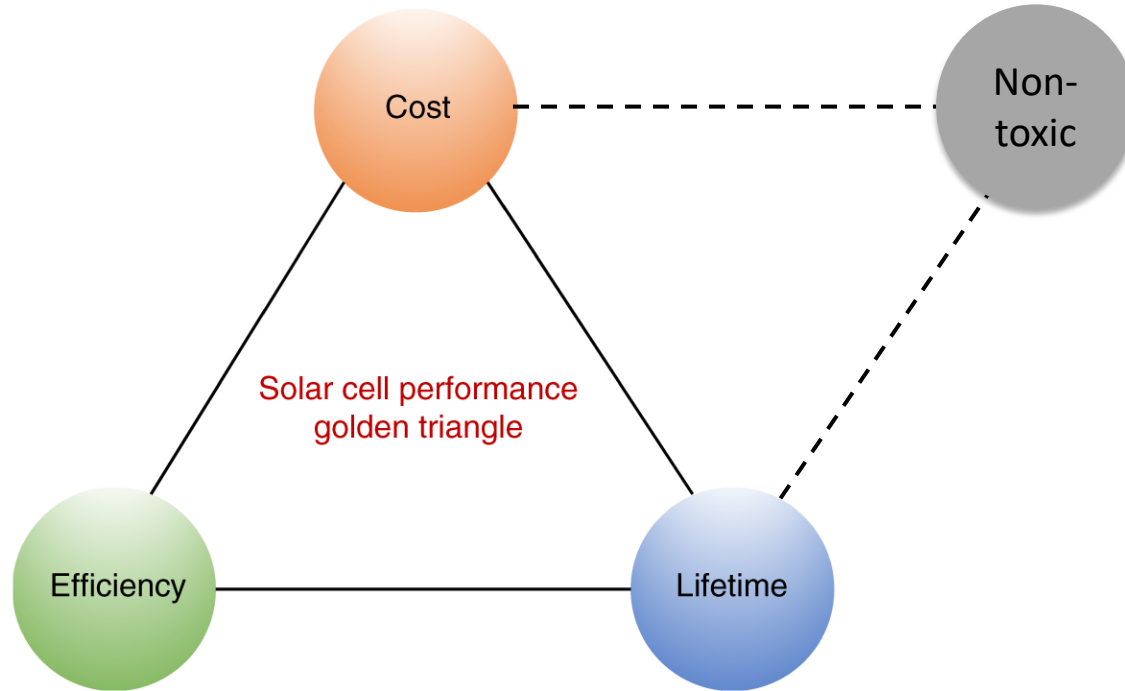
- Performance: [High efficiency](#)  
Production Cost: [Low](#)  
Fabrication : [Simple](#)  
Others: [Flexible](#)  
[Portable](#)  
[Light-weight](#)



<http://gcell.com/>



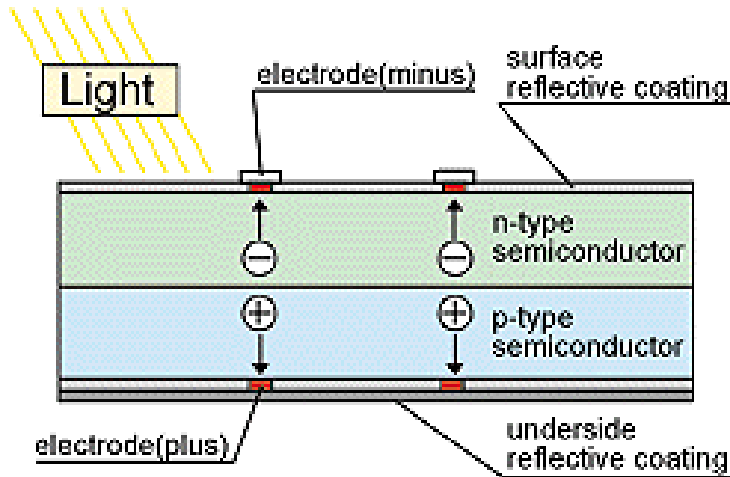
# Golden Triangle



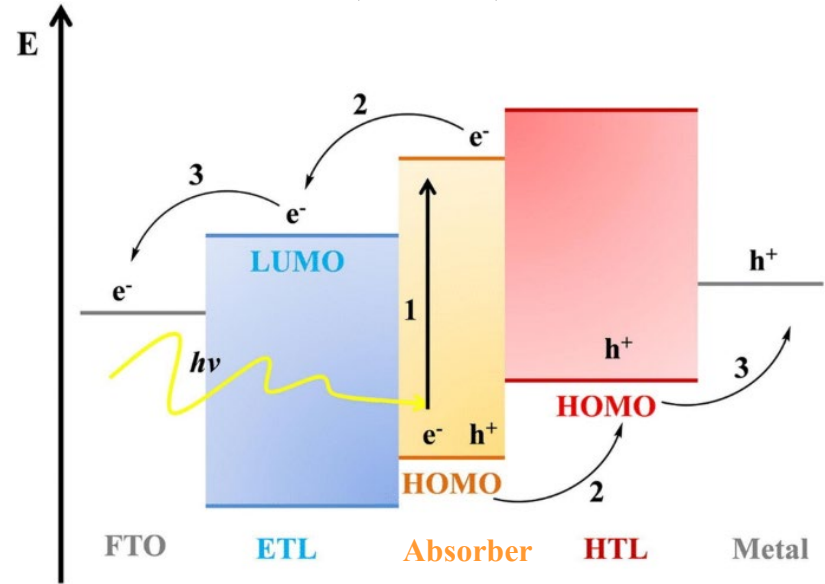
<https://www.nature.com/articles/s41467-018-07255-1>

# Working Principle of Solar Cells

## Heterojunction solar cells



## PSCs, OPV, DSSCs etc

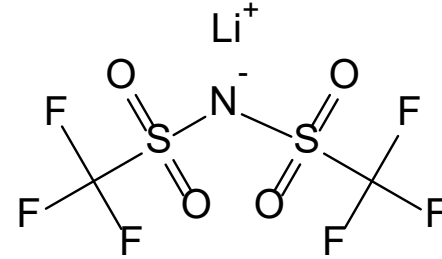
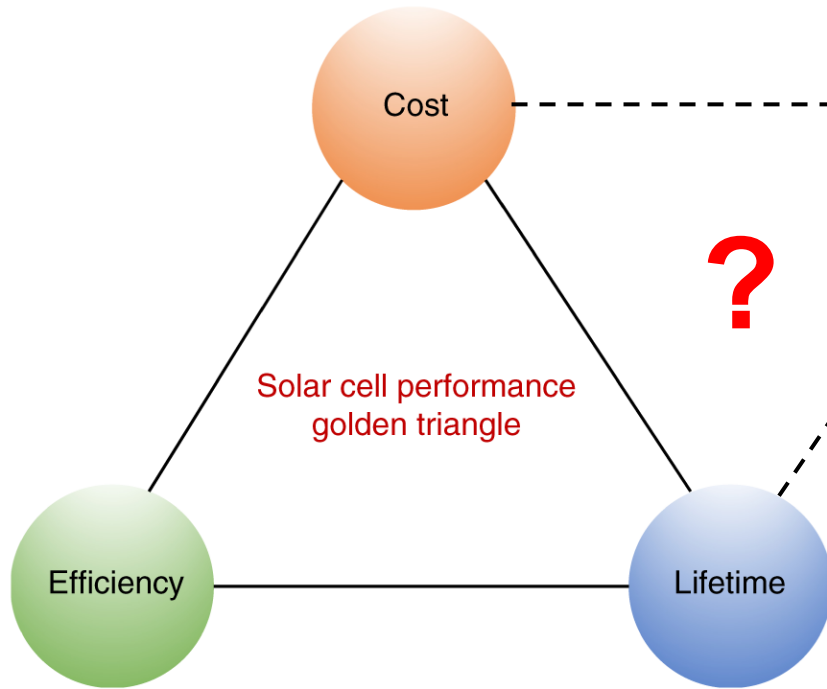


The role of hole transporting materials is to efficiently select and transport the photogenerated holes.

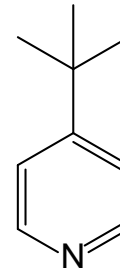
**HTM should be *p*-type semiconductor.**



# Hole Transporting Materials

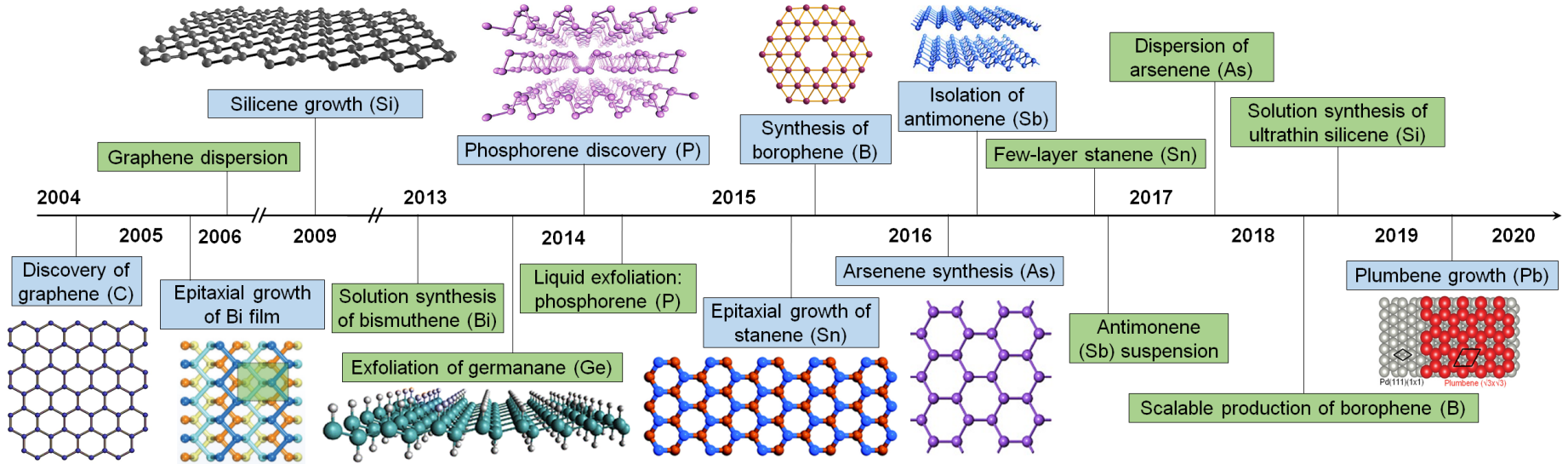


Lithium bis-(trifluoromethanesulfonyl)imide (LiTFSI)



4-tertbutyl pyridine (4-tBP)

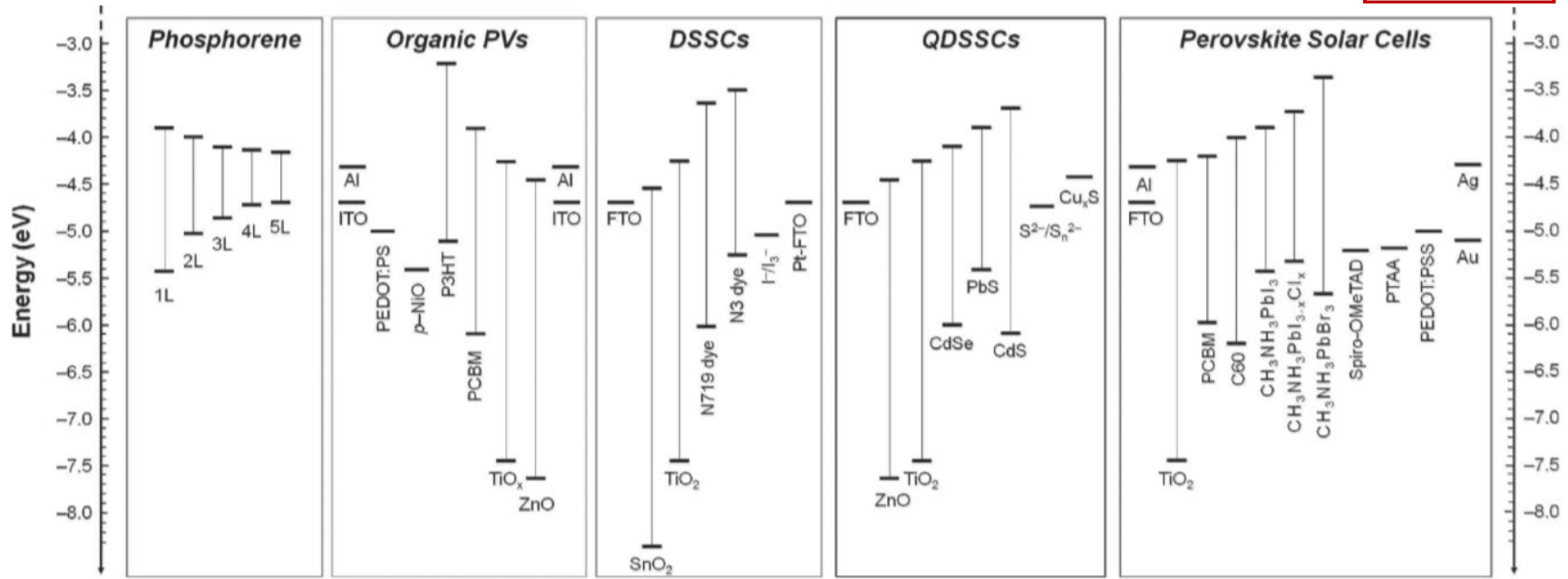
# Development of 2D Materials



(MJ) Bat-Erdene et al. *Adv Funct Mater.*, **2022**, 32, 2107280.

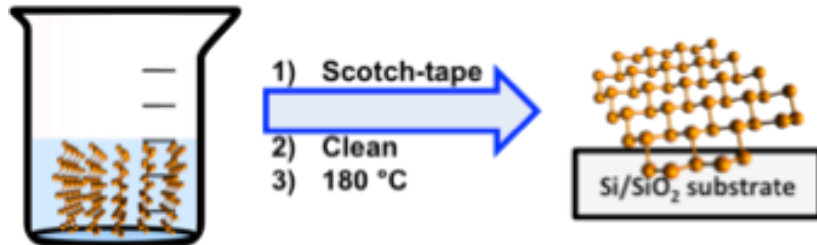
# 2D Black Phosphorus (BP)

Type	Phosphorene
	Semiconductor
Bandgap (eV)*	0.3 – 2.0
Carrier mobility, (cm <sup>2</sup> V <sup>-1</sup> s <sup>-1</sup> )	≈1000
ON/OFF ratio	10 <sup>3</sup> – 10 <sup>5</sup>
Thermal conductance (W m <sup>-1</sup> K <sup>-1</sup> )	10 – 36
Thermoelectric performance, ZT	1 – 2.5



Batmunkh et al. *Adv. Mater.*, **2016**, 28, 8586.  
 Batmunkh et al. *Adv. Energy Mater.*, **2017**, 1701832.

# Conventional Preparation Methods (Phosphorene)



## Mechanical Exfoliation (Scotch-Tape)

- Poor scalability
- Low production yield
- Instability



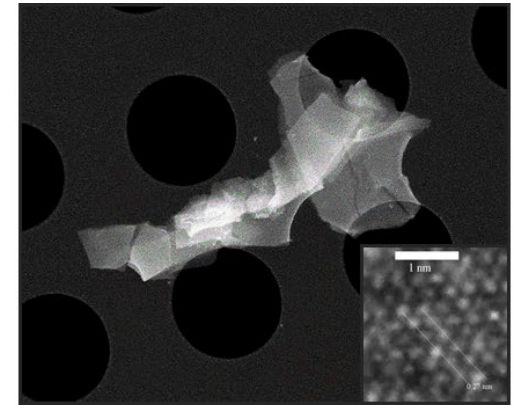
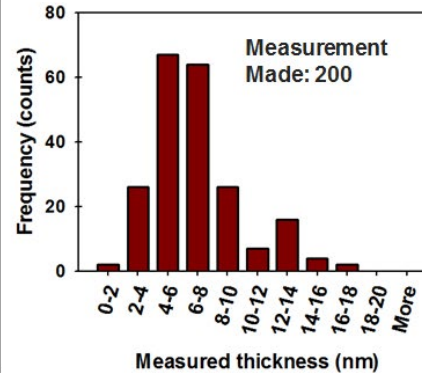
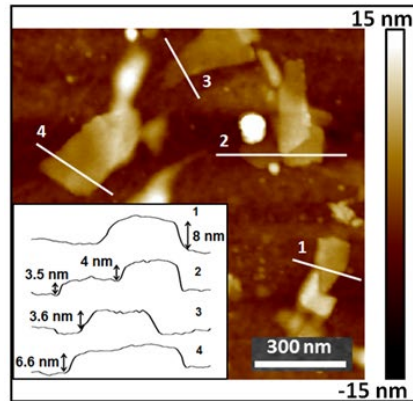
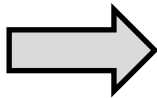
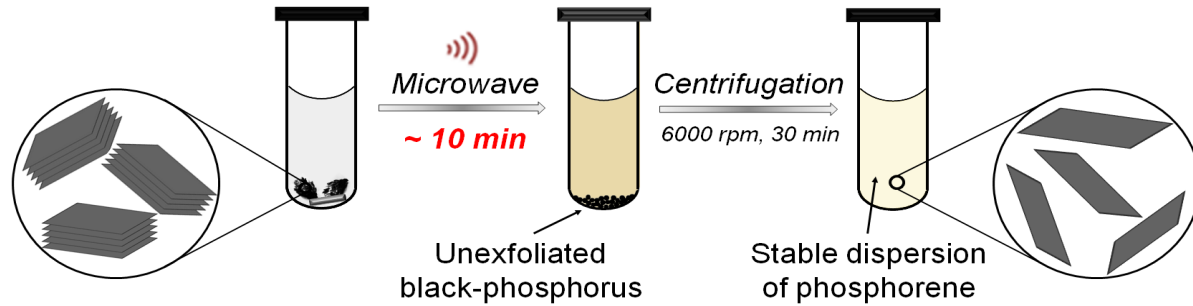
## Sonication Based Liquid-Exfoliation

- Long processing time (~20 h)
- Damage to the flakes
- Poor quality

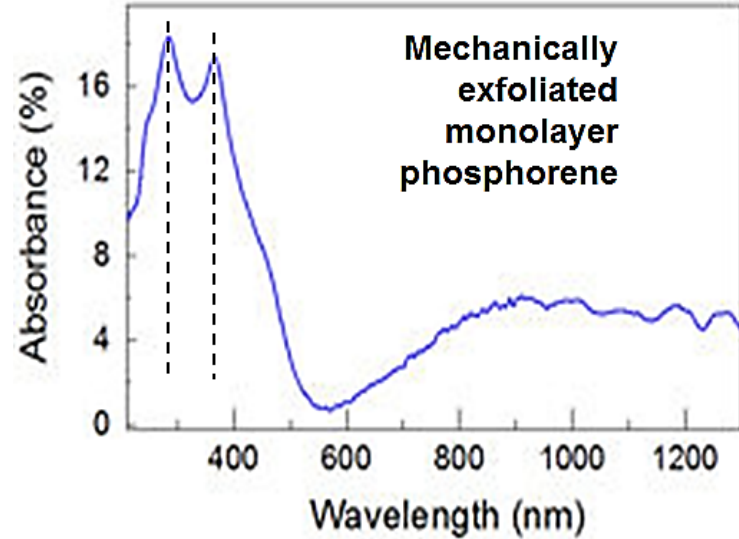
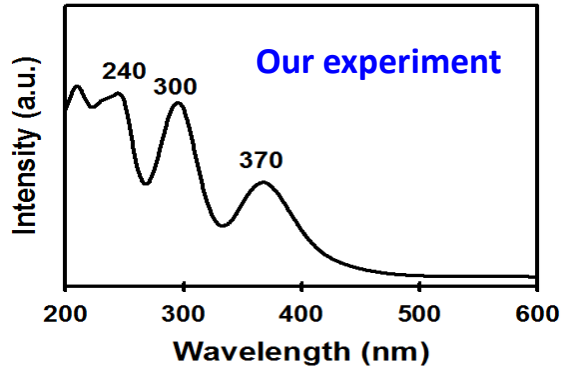
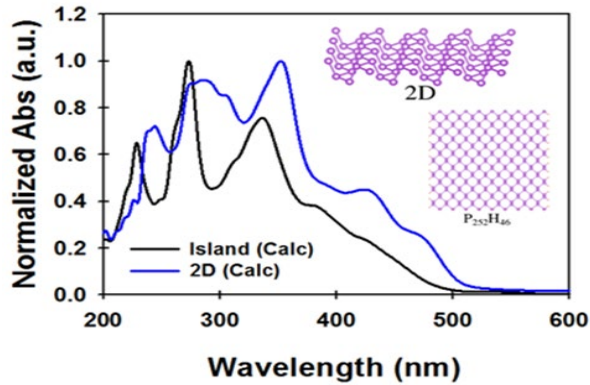
Li et al. *Nat Nanotechnol*, 2014, 9, 372.

Yasaei et al. *Adv. Mater*, 2015, 27, 1887.

# Microwave-Assisted Preparation (Phosphorene)

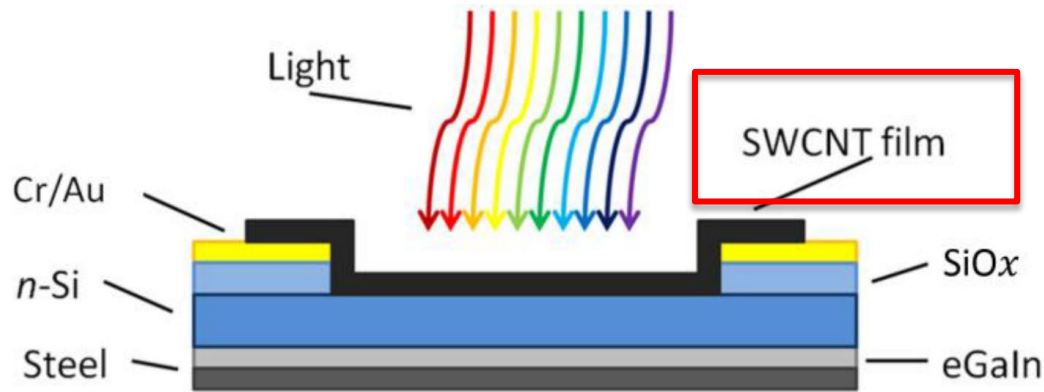


# Microwave-Assisted Preparation (Phosphorene)



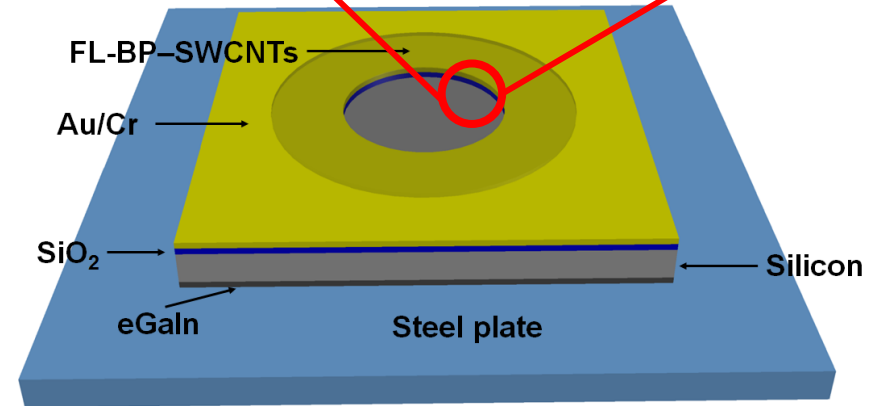
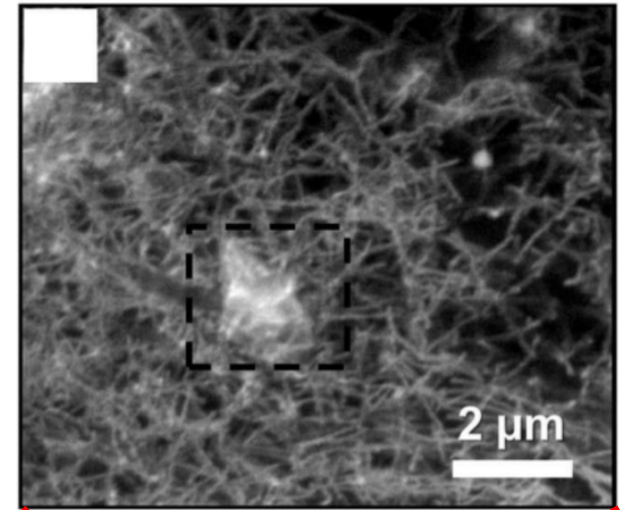
*NPJ 2D Mater & Appl.*  
2017, 1, 18.

# Si-CNTs Solar Cells



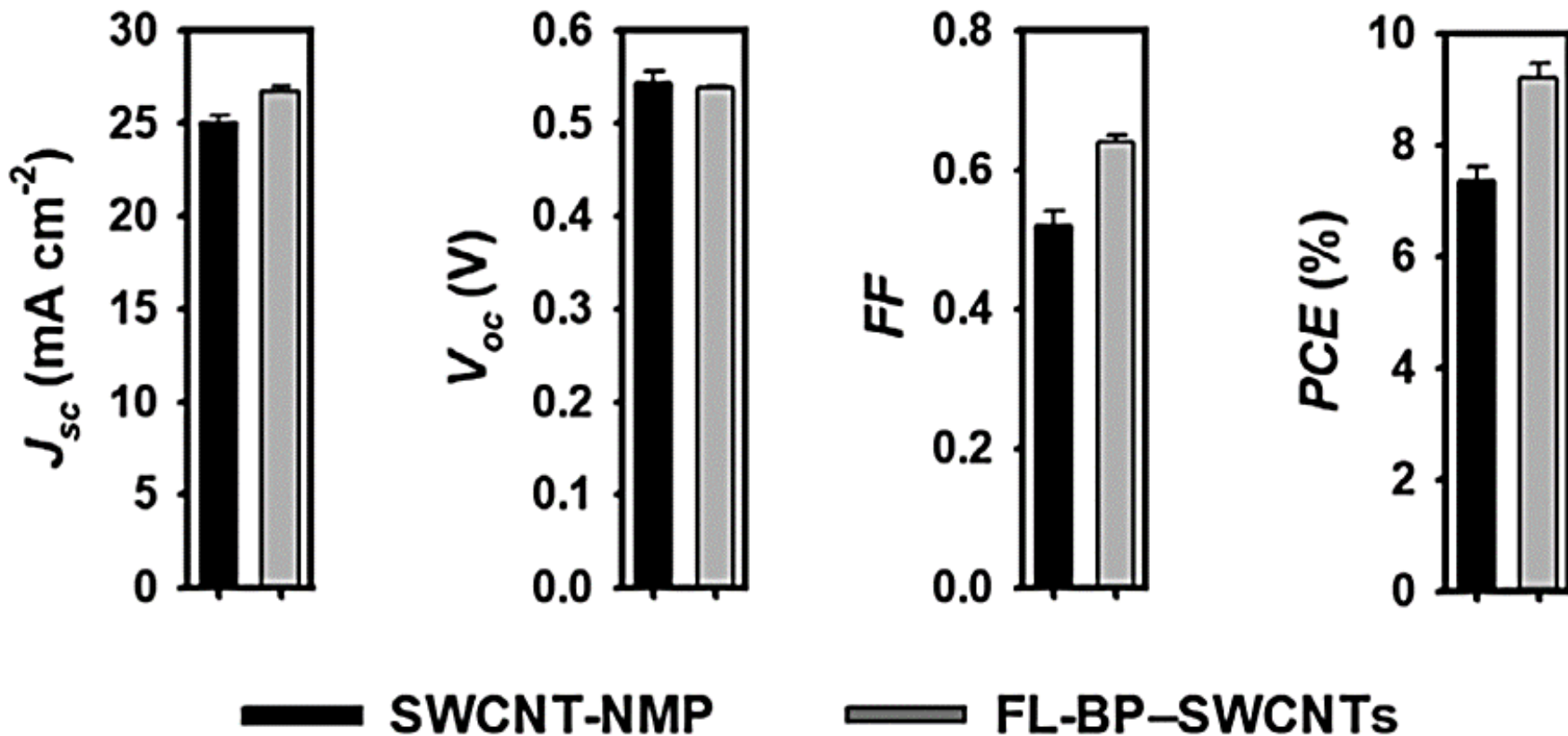
## Disadvantages of CNTs:

- Formation of sparse network
- Poor hole selectivity

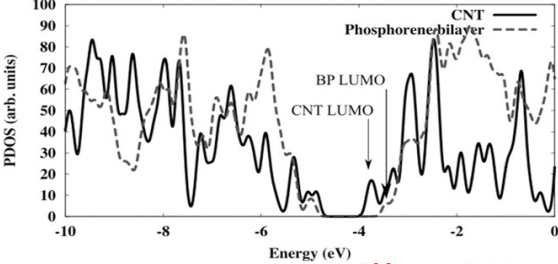
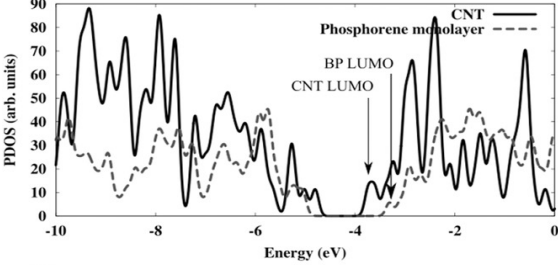
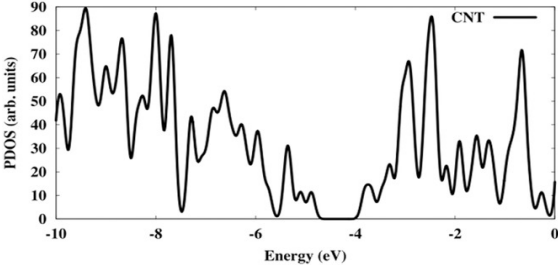
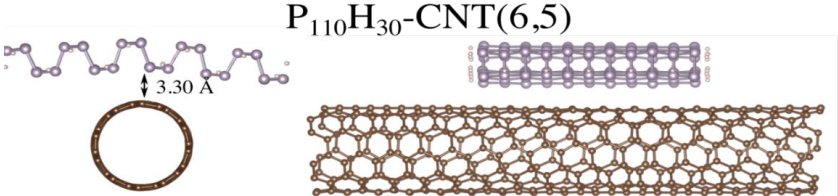
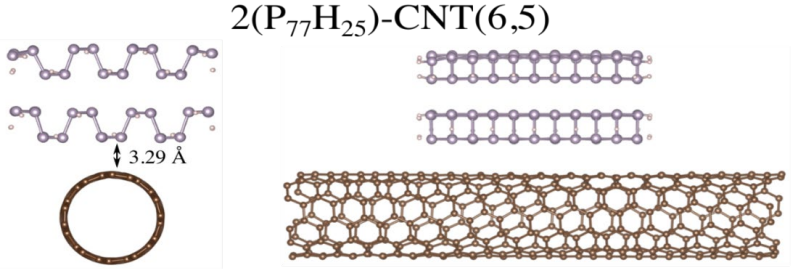
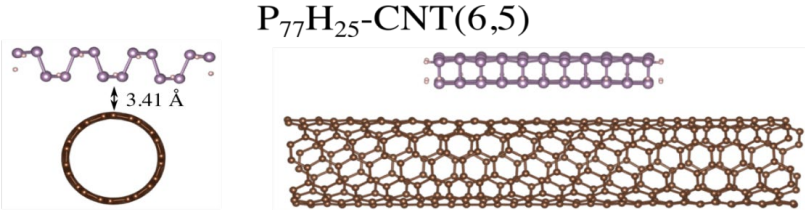




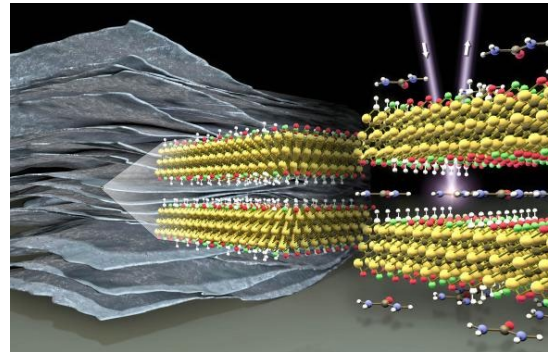
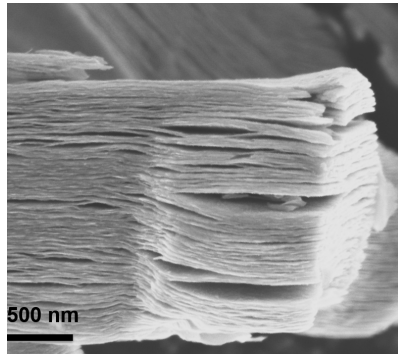
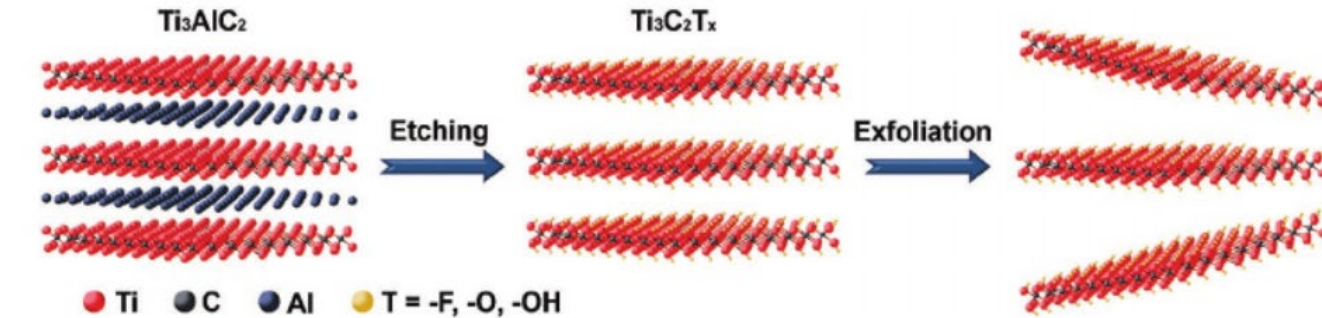
## Si-CNTs Solar Cells



# Si-CNTs Solar Cells

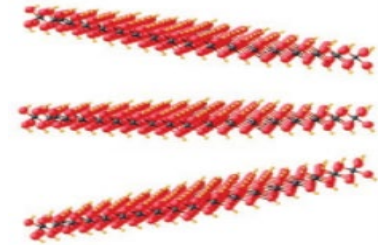
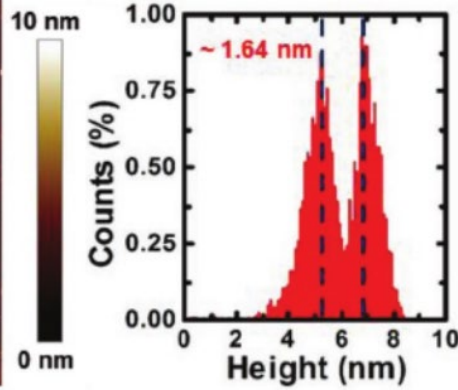
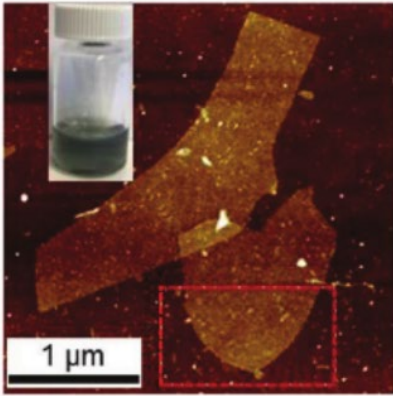


# MXene ( $\text{Ti}_3\text{C}_2\text{T}_x$ )

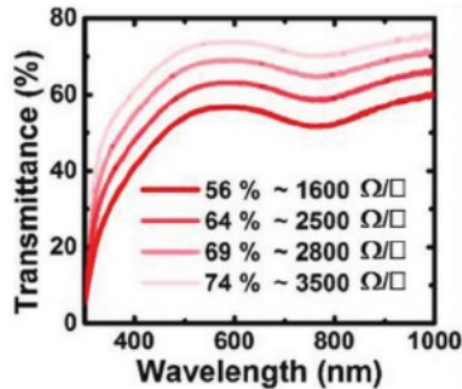
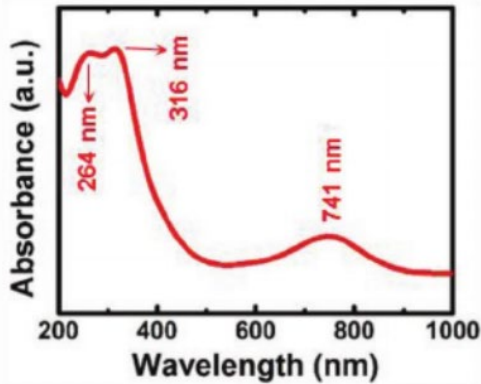


Yu and Bati *et al.* *Adv. Energy Mater.* **2019**, 9, 1901063.

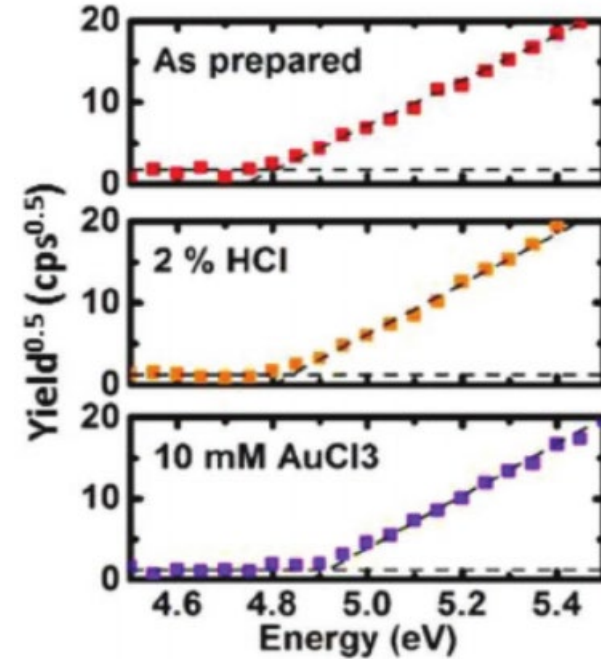
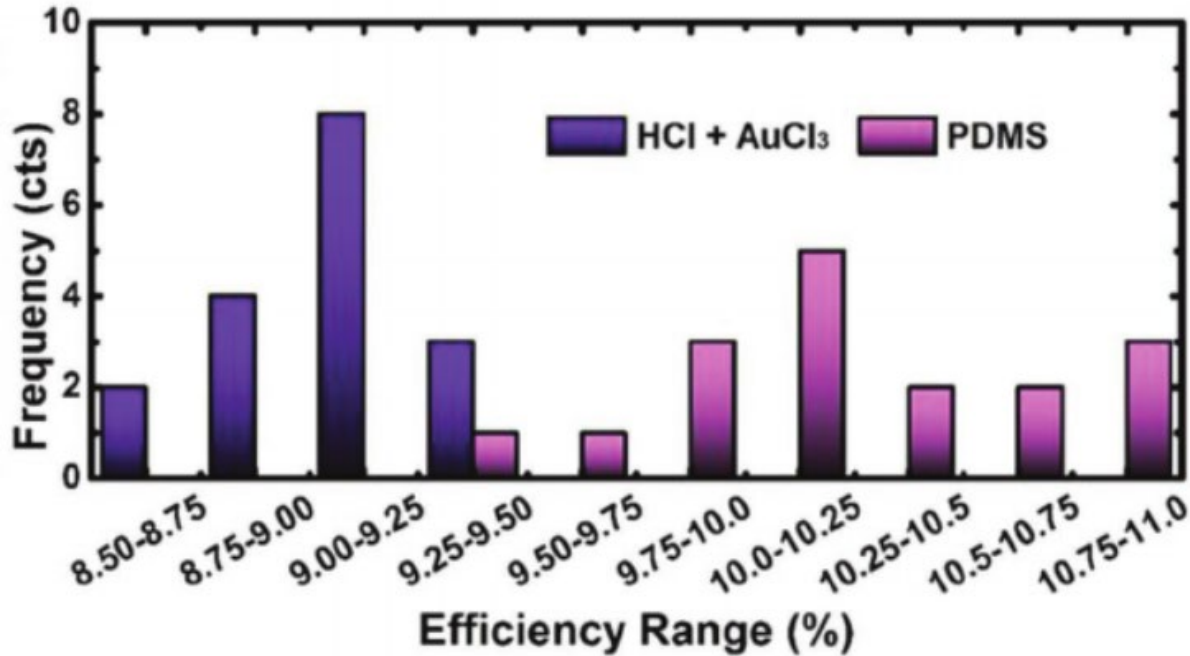
# n-Si/MXene Heterojunction



n-Silicon

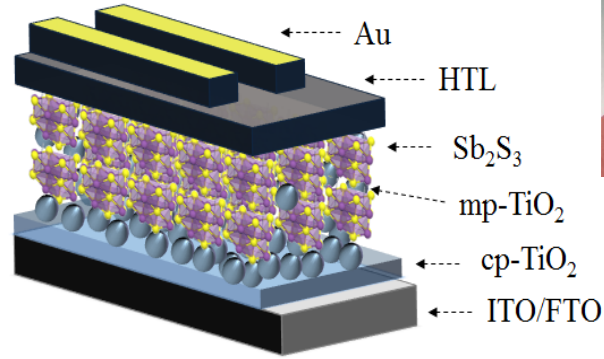
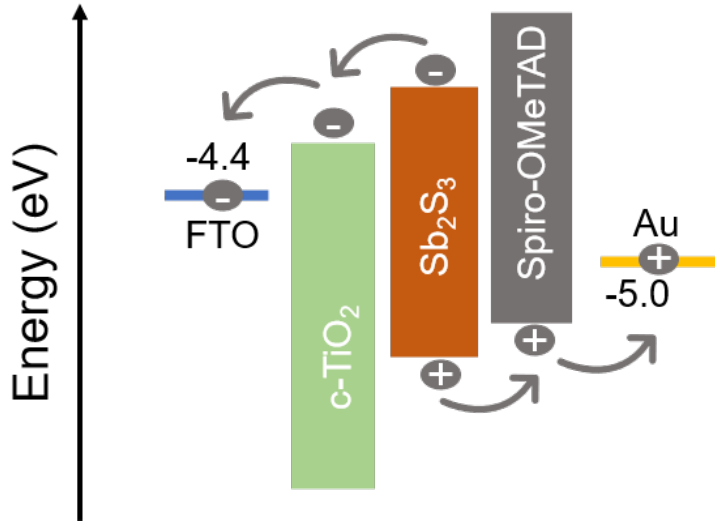


# n-Si/MXene Solar Cells

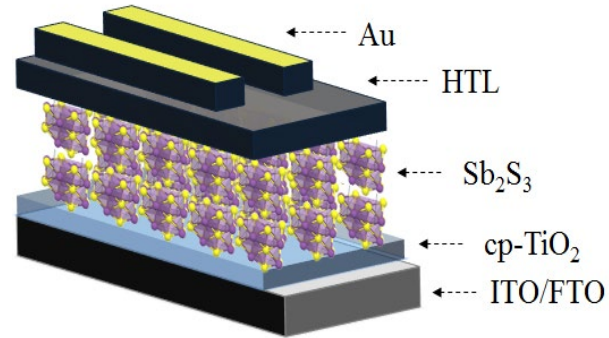




# Sb<sub>2</sub>S<sub>3</sub> solar cells



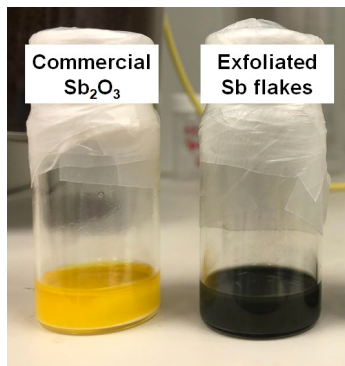
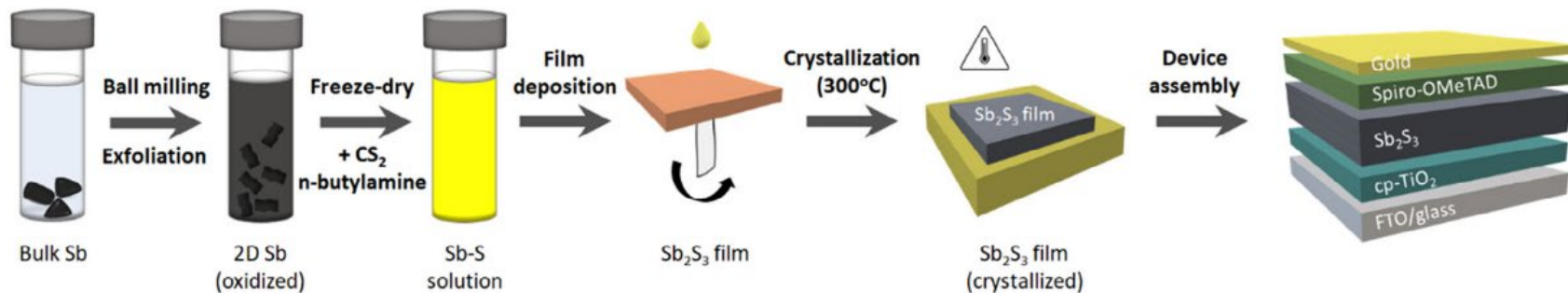
Mesoporous Sb<sub>2</sub>S<sub>3</sub> solar cells



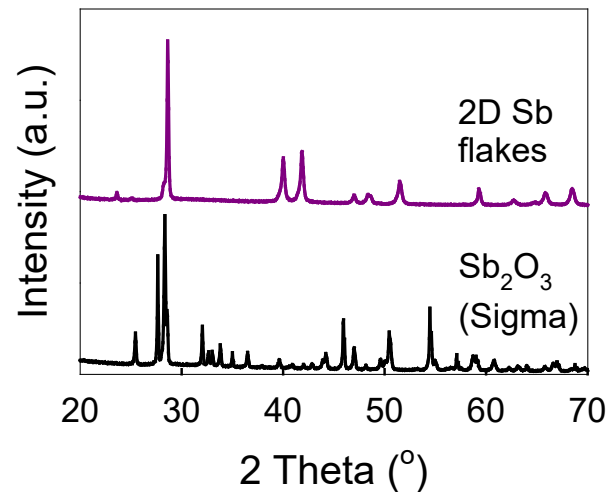
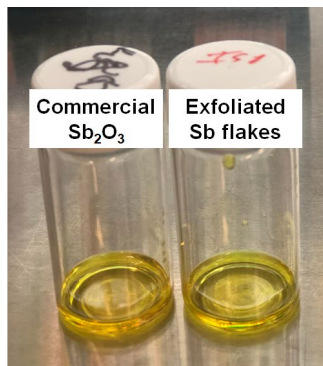
Planar Sb<sub>2</sub>S<sub>3</sub> solar cells



# Making $\text{Sb}_2\text{S}_3$ Solar Cells

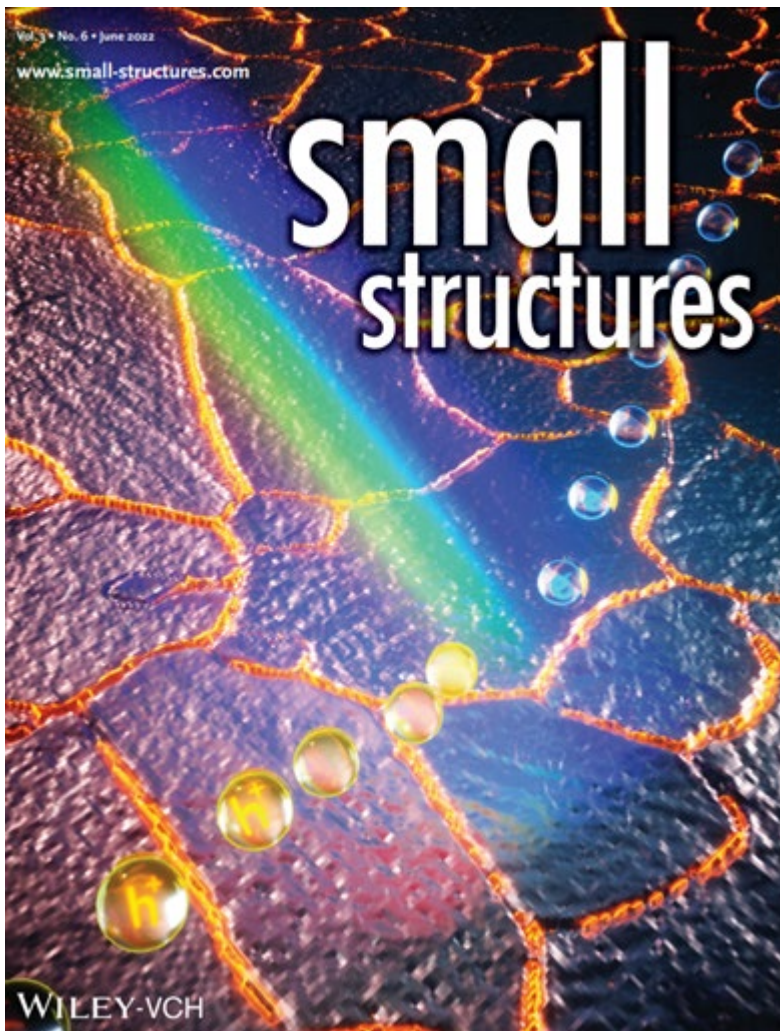


Stirring

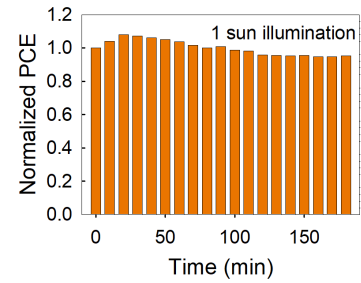
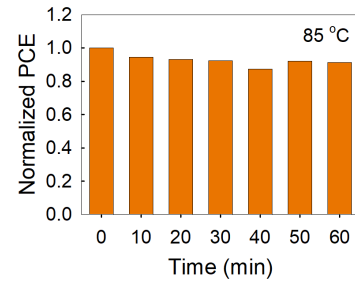
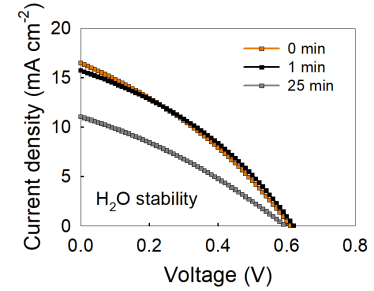
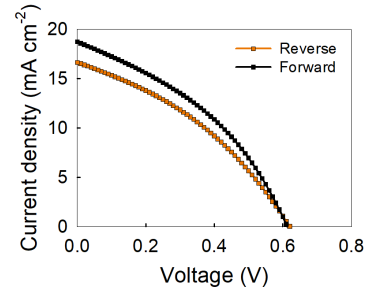
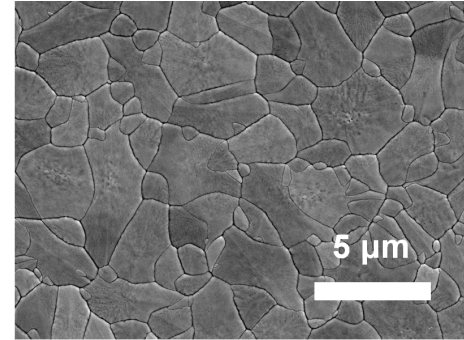


(MJ) Bat-Erdene et al. *Small Structures.*, **2022**, 3, 2200038.



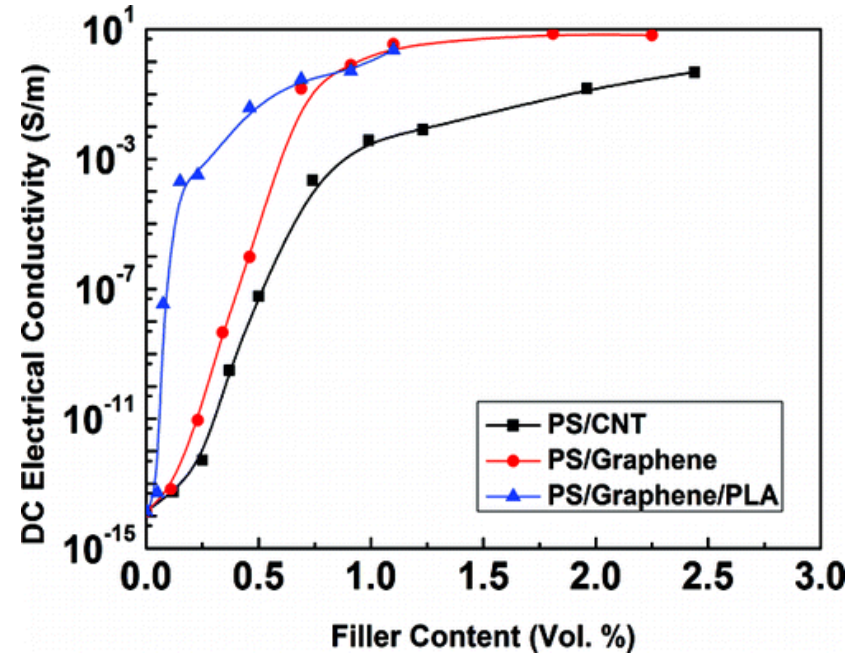


Crystallized in Air +  
Glovebox (>2 min)



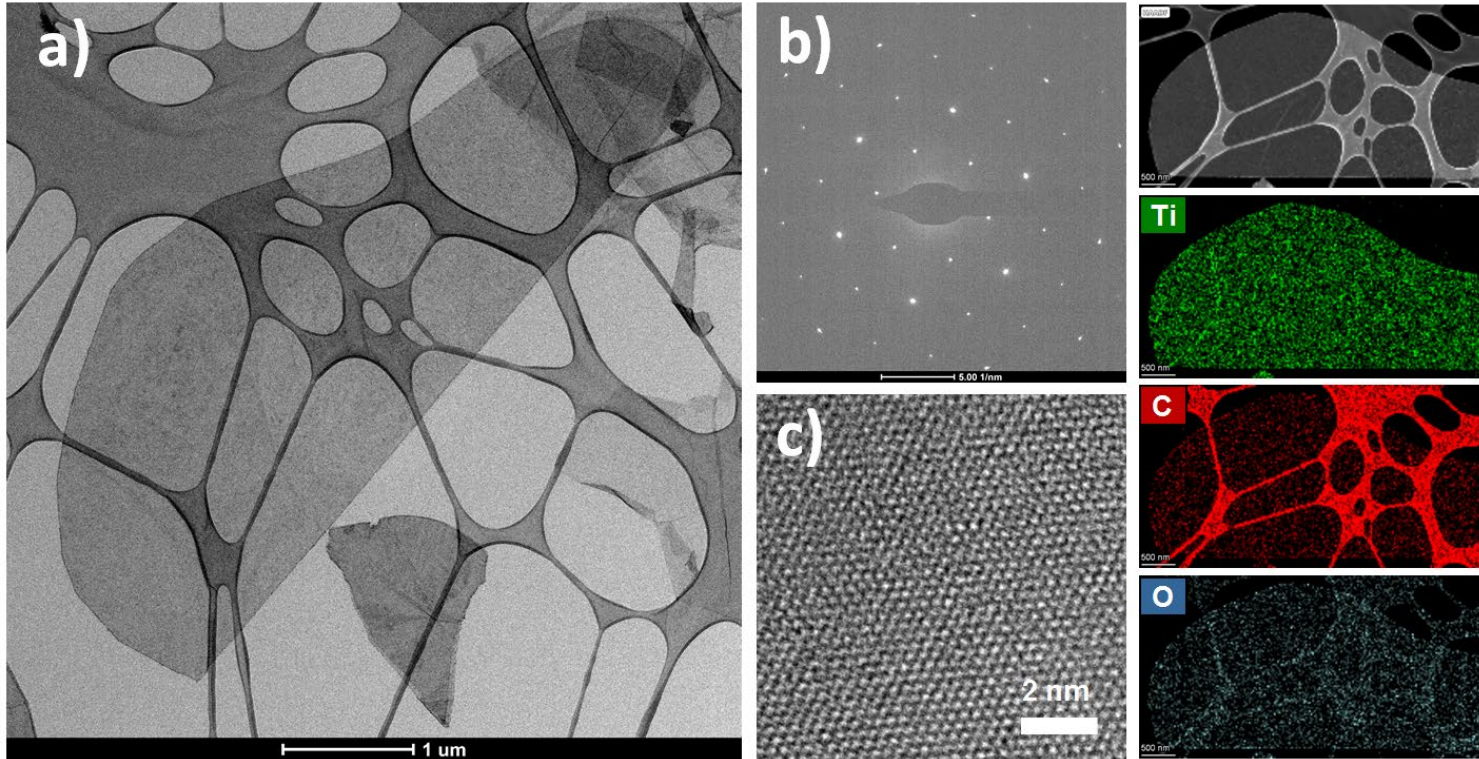
# ***PEROVSKITE SOLAR CELLS***

# Polystyrene – insulator

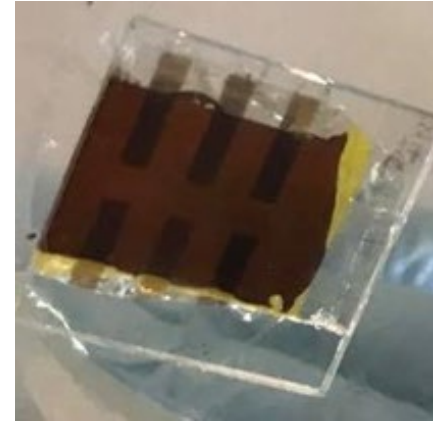
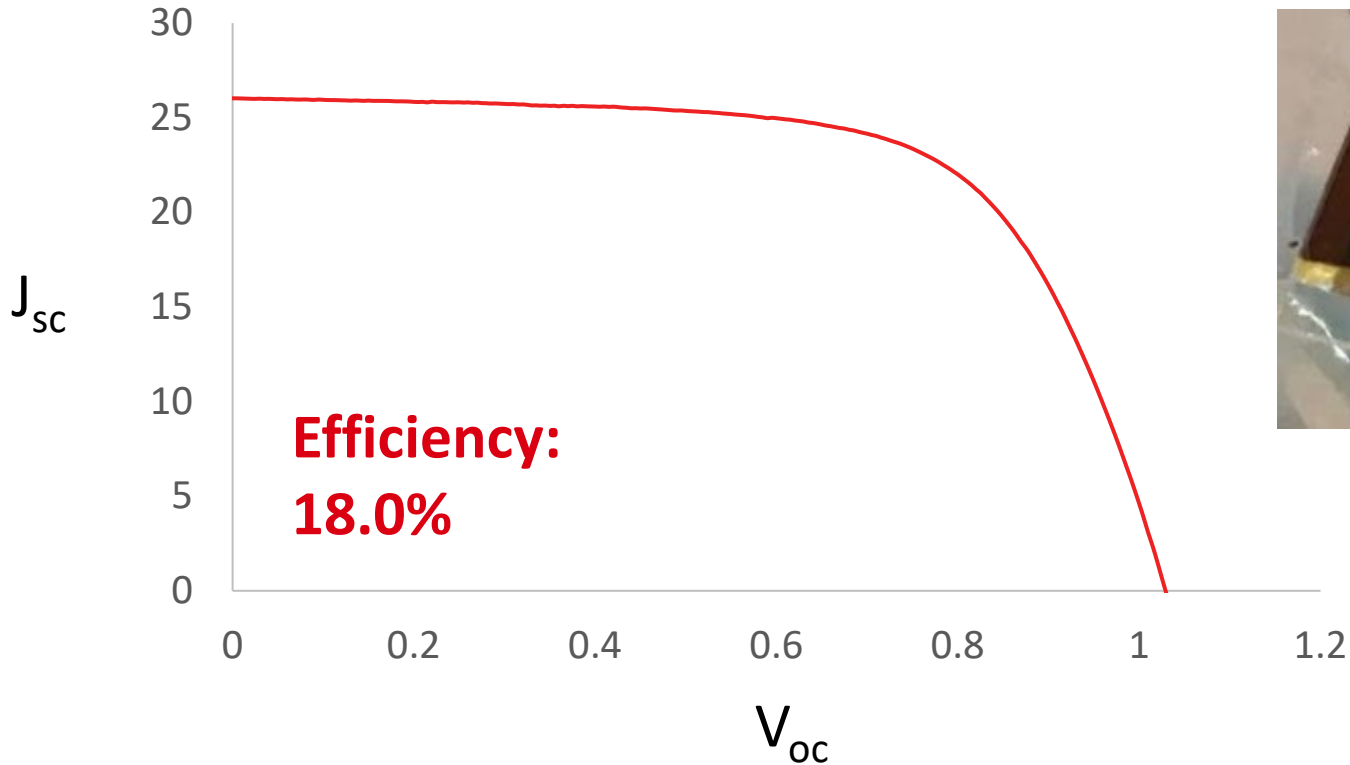




# MXene ( $Ti_3C_2T_x$ )



# MXene ( $Ti_3C_2T_x$ )-PS for Perovskite Solar Cells In ambient air



# Conclusion

2D materials such as MXene, black phosphorus and graphene are promising candidates as p-type hole selective and conductive materials for solar cells.

A lot still remains to be done in the development of facile, cost-effective, scalable and green production methods for these 2D materials.

Many thanks to:



**Australian Government**  
**Australian Research Council**



**MICROSCOPY  
AUSTRALIA**



ANFF



  
**THE UNIVERSITY  
of ADELAIDE**



**THE UNIVERSITY  
OF QUEENSLAND**  
AUSTRALIA  
CREATE CHANGE



 **Griffith** UNIVERSITY  
Queensland, Australia

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(Prof Joe Shapter's group)

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Prof Tianyi Ma (RMIT)

Dr Cameron Shearer (Univ of Adelaide)

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Dr Abdulaziz Bati (UQ)

Dr Md J Nine (Univ of Adelaide)

Prof Sarangerel (Nat Univ of Mongolia)



THANK YOU

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