Striving for Excellence: Experience Publishing in Nature Materials (IF 38.9)

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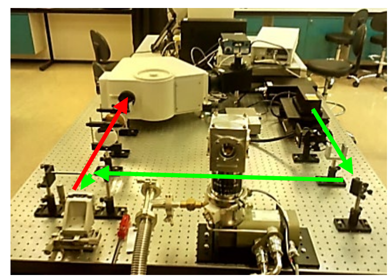
IMEN UKM

Research themes:

- MEMS/NEMS & Nanoelectronics
- Organic & Printed Electronics
- Photonics & Nanophotonics
- Microelectronics Semiconductor Packaging
- Micro & Nanoelectronics System



BH ONLINE

BERITA SUKAN DUNIA HIBURAN BISNES RENCANA WANITA HUJUNG MINGGU BH KAPSUL

BERITA » Pendidikan
Selasa, 27 Ogos 2019 | 6:41pm

Naib Canselor UKM, Prof Ir Dr Mohd Hamdi Abd Shukor (kiri) bersama penyelidik IMEN, Dr Abdul Rahman Mohamd pada sidang media khas penyelidikan UKM berjaya menerbit dalam Jurnal Nature Materials di UKM Bangi. - NSTP/Rohanis Shukri

Penyelidik UKM muncul saintis pertama pengarang jurnal Nature Materials

Oleh Halina Mohd Noor
halina_mdnoor@bh.com.my

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BANGI: Penyelidik Institut Kejuruteraan Mikro dan Nanoelektrik (IMEN), Universiti

Outline

- Research journey
  - PhD study at University of Sheffield, UK
  - Transition from PhD to academia
  - Postdoctoral experience at Rutgers University, US
- Our findings & publishing in Nature Materials
  - Application and demands for hydrogen
  - 2D Transition Metal Dichalcogenides (TMDs) catalyst for hydrogen evolution
  - Key results
- Work Life Balance

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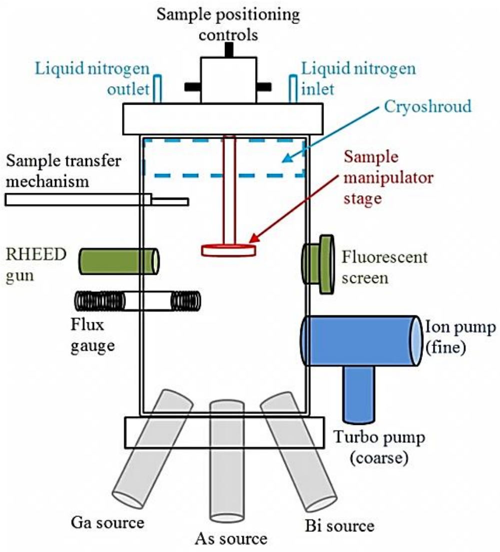
PhD journey

- PhD at University of Sheffield, UK
- Joined a big group (~20 PhD students + 4 postdocs)
- Worked on MBE growth and characterization of III-V semiconductors ($GaAs_{1-x}Bi_x$)

Material	Thickness (nm)
GaAs cap	80
$GaAs_{1-x}Bi_x$ layer	160
GaAs buffer	80
S.I (100) GaAs substrate	

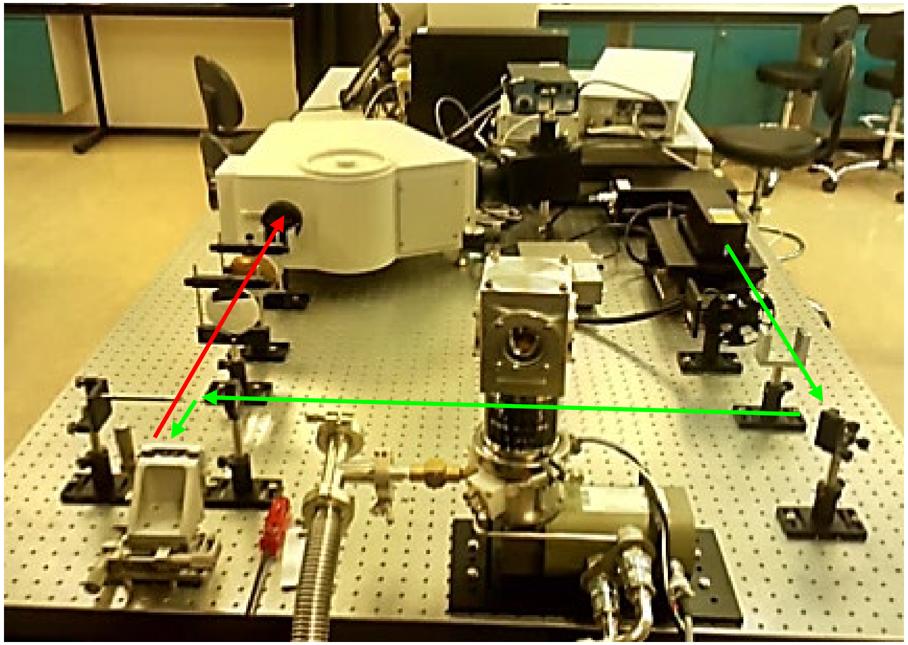


PhD journey

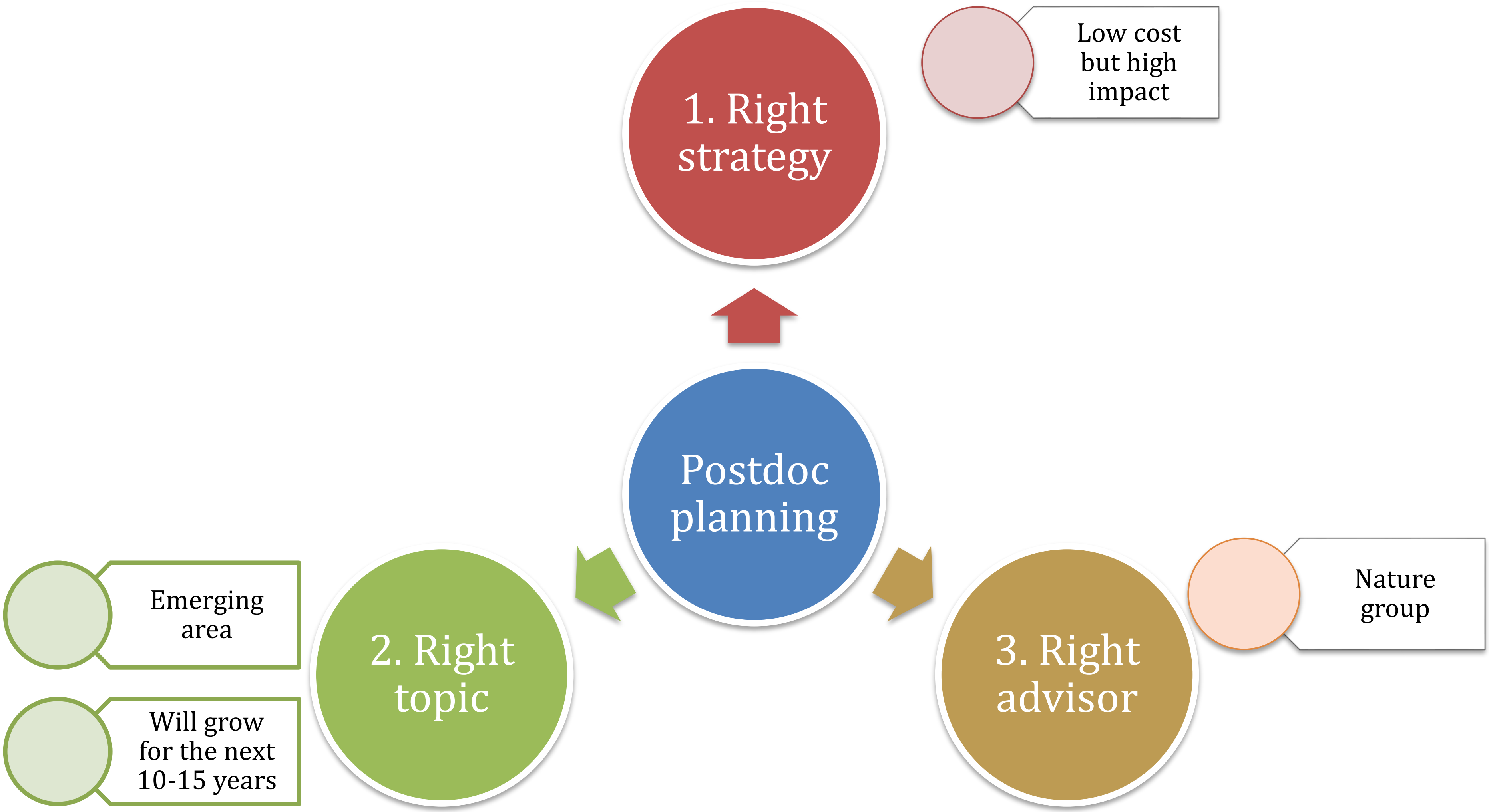
- Graduated with 7 journals (5 as the first author)
- 5 Q1s including 3 publications in Applied Physics Letters (Q1, IF 3.5)
- Attended 5 conferences in USA, Japan, German, Finland and UK.

Transitional period

- MBE is expensive growth method
- Peer pressure
- Focusing on material characterizations
- The unexpected inspiration



The three-rights (3Rs)



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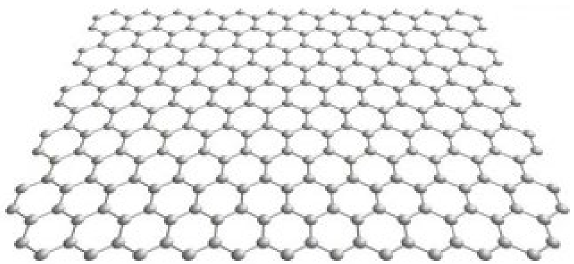
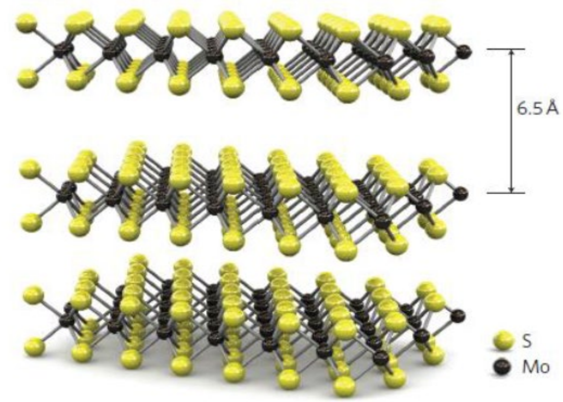
Choosing the right topic



Graphene

versus



Properties of TMDs, MX_2, are diverse – insulators (HfS_2), semiconductors (MoS_2) , metals (NbS_2, VS_2) etc.

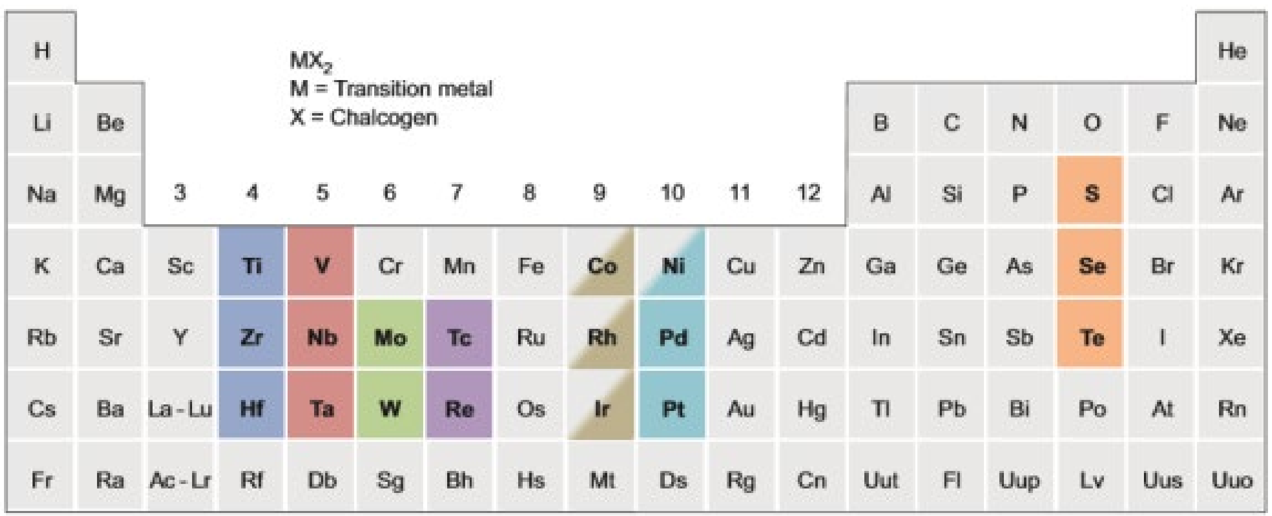


Table 1 | Electronic character of different layered TMDs[25].

Group	M	X	Properties
4	Ti, Hf, Zr	S, Se, Te	Semiconducting (E_g = 0.2–2 eV). Diamagnetic.
5	V, Nb, Ta	S, Se, Te	Narrow band metals (ρ ~ 10^{-4} Ω.cm) or semimetals. Superconducting. Charge density wave (CDW). Paramagnetic, antiferromagnetic, or diamagnetic.
6	Mo, W	S, Se, Te	Sulfides and selenides are semiconducting (E_g ~ 1 eV). Tellurides are semimetallic (ρ ~ 10^{-3} Ω cm). Diamagnetic.
7	Tc, Re	S, Se, Te	Small-gap semiconductors. Diamagnetic.
10	Pd, Pt	S, Se, Te	Sulfides and selenides are semiconducting (E_g = 0.4 eV) and diamagnetic. Tellurides are metallic and paramagnetic. $PdTe_2$ is superconducting.

ρ, in-plane electrical resistivity.

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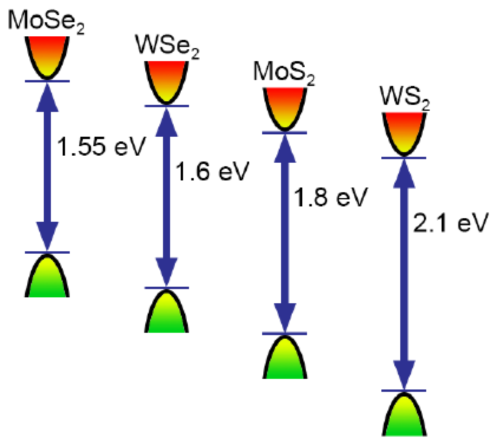
Choosing the right topic

- Properties of 2D TMDs are diverse. Plenty of things to study!



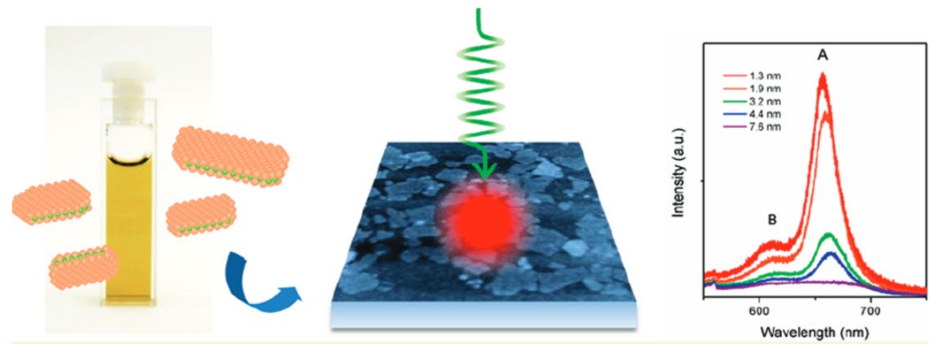
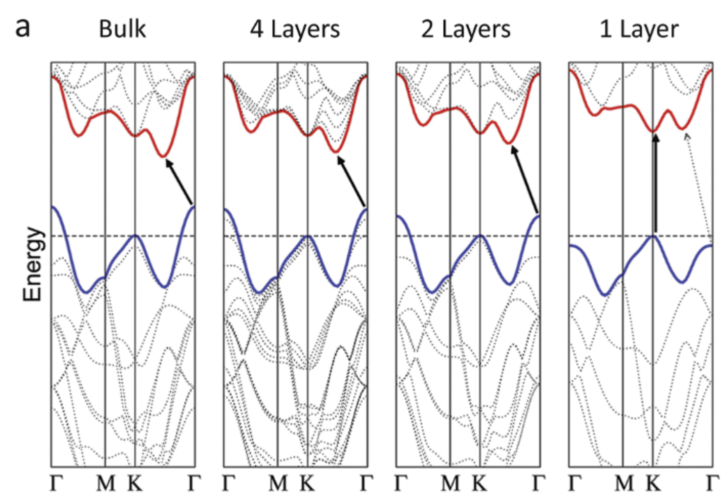


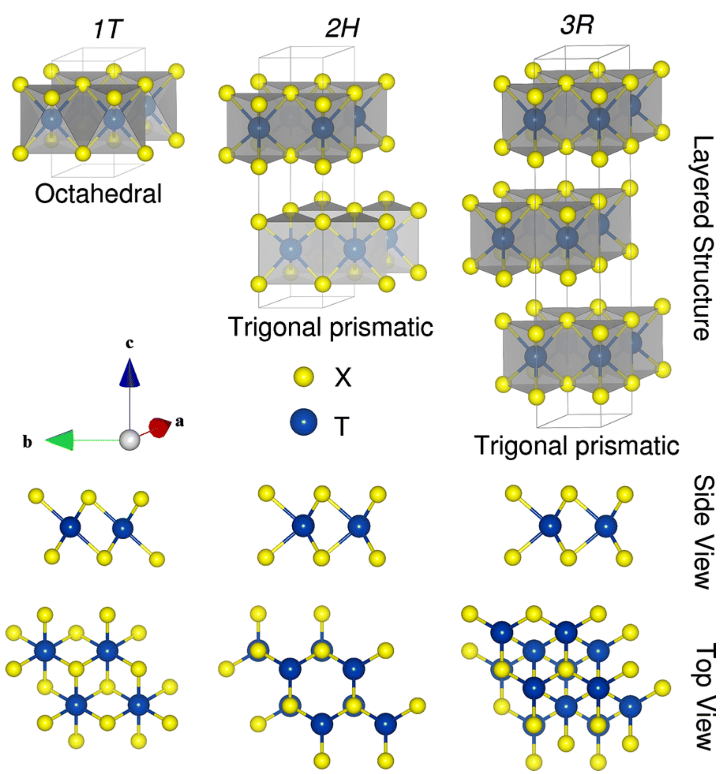
Table 2.1: Band gaps of bulk and single layer LTMD semiconductors

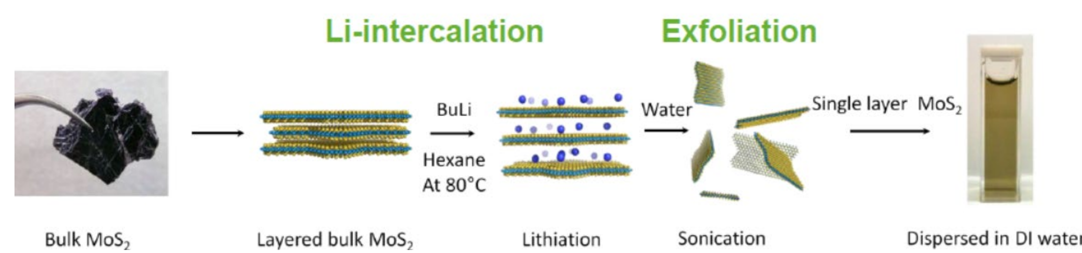
LTMD	Bulk band gap (eV)	Single layer band gap(eV)
$MoTe_2$	1.0	1.1
$MoSe_2$	1.1	1.5
WSe_2	1.2	1.6
MoS_2	1.2	1.8
WS_2	1.4	2.1
SnS_2	2.1	2.2



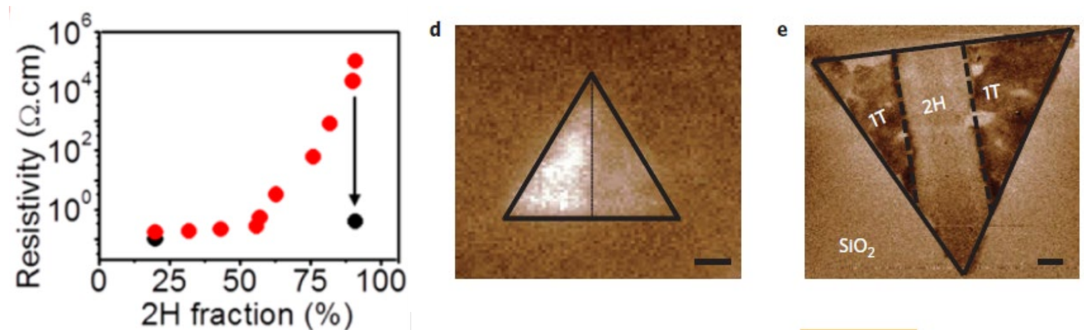
Choosing the right topic

- Phase engineering – 2H to 1T MoS2 (looks interesting!)

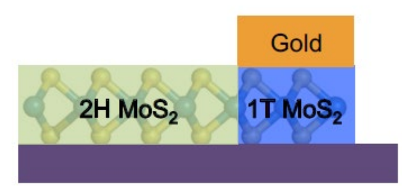




Acerce, Nature Nano (2015)



Eda, Nano Lett. (2011)



Scouting for potential advisor

- Target to join 'Nature group'

Prof. Ajayan Pulickel
Rice Uni, USA
Citations: 99,800
H-index: 152

Prof. Manish Chhowalla
Rutgers Uni, USA
Citations: 48,000
H-index: 86

Prof. Jing Kong
MIT, USA
Citations: 43,000
H-index: 100

Prof. Andras Kis
EPFL, Switzerland
Citations: 30,600
H-index: 48

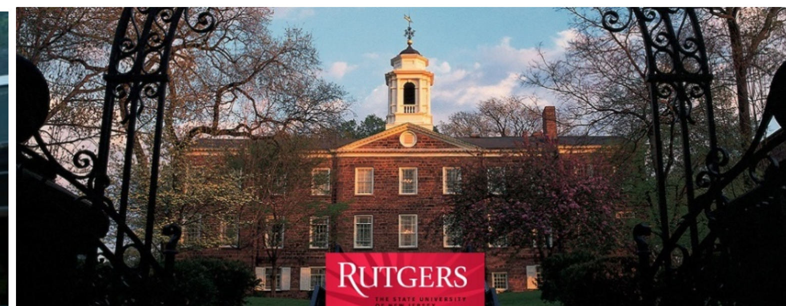
Dr. Goki Eda
NUS, Singapore
Citations: 27,000
H-index: 50

Prof. Jamie Warner
Oxford Uni, UK
Citations: 9,600
H-index: 49

Postdoc at Rutgers

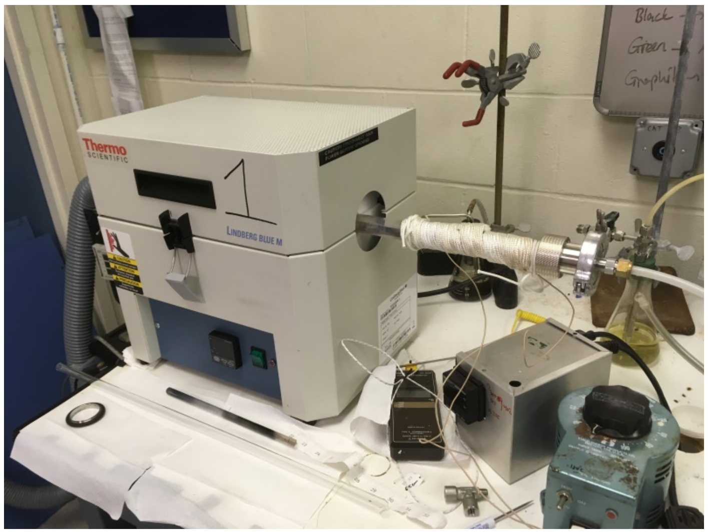
- 2 years in Rutgers from Jan 2016 to 2018
- Members: 5 students + 1 postdoc (+2 PDs & few students)
- Main activities are chemistry related!

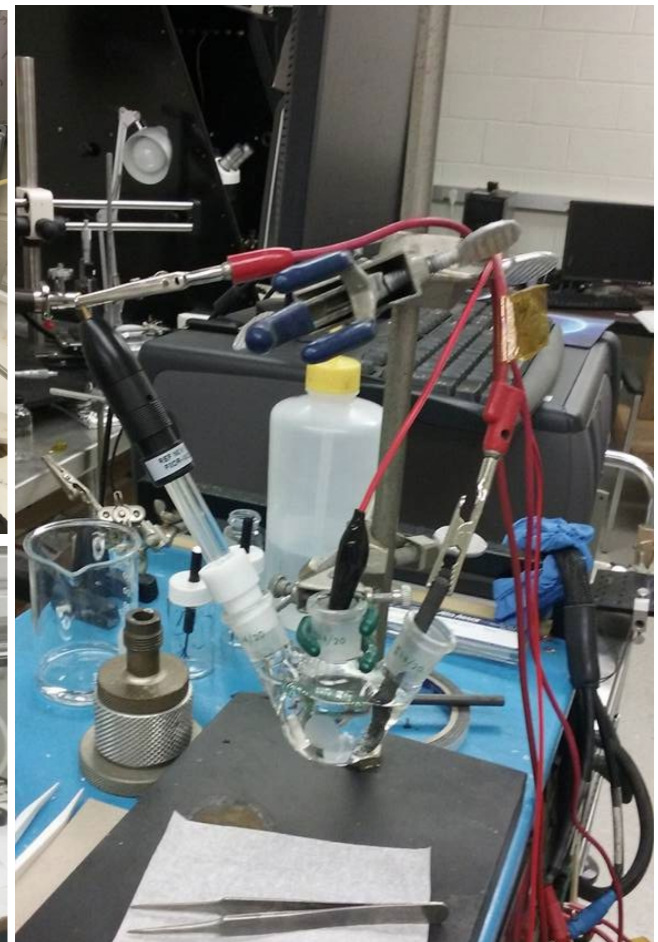
UTM #217, UKM #160, RUTGERS #262



Postdoc at Rutgers

- Equipments and lab facilities





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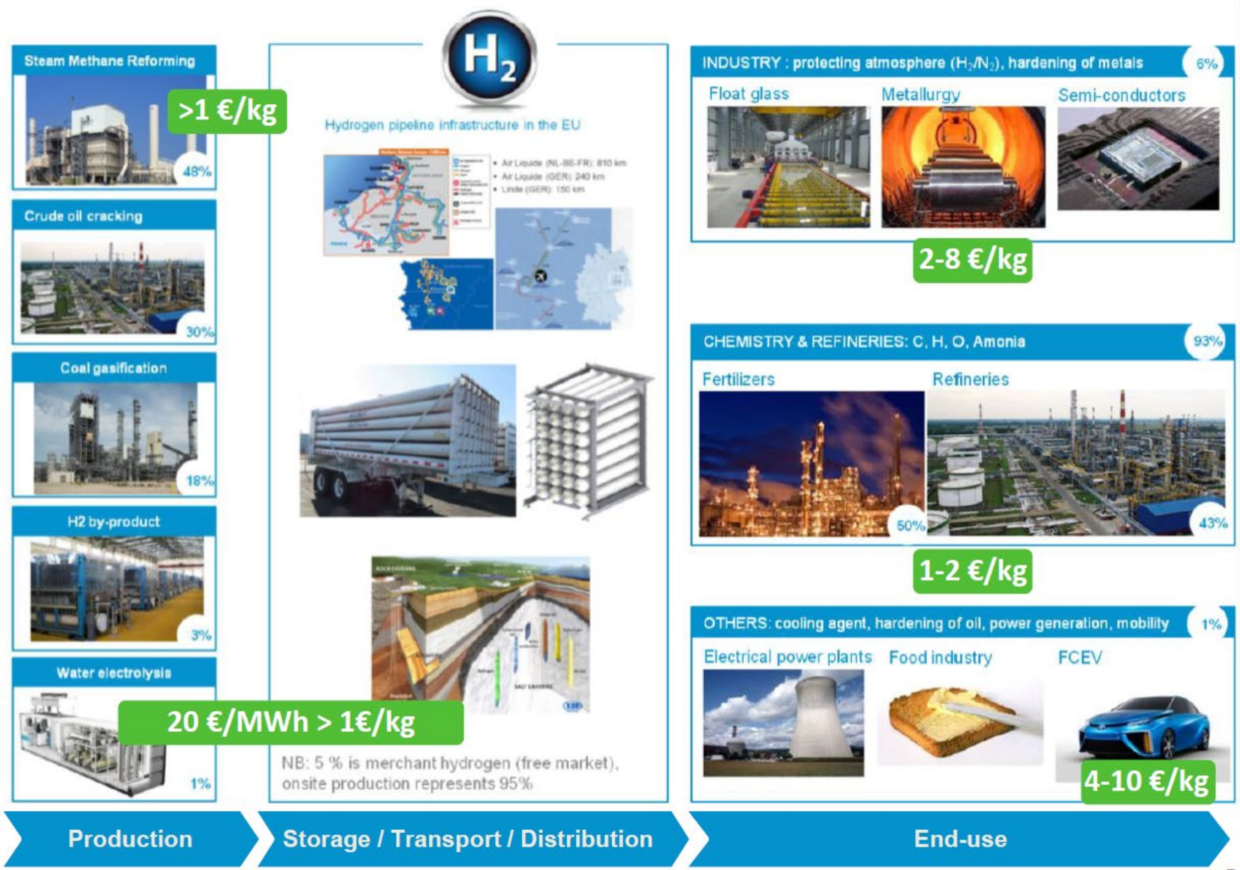
Hydrogen market

- In 2017, hydrogen generation market was valued ~$115 billion and is expected to grow to $155 billion in 2020.



But most (96%) of the hydrogen produced today is not CO_2-free (from gas, oil, coal)

⇩

If produced from renewable power via electrolysis, hydrogen is fully renewable and CO_2-free.

⇩

Renewable hydrogen has the potential to decarbonize a large range of applications

Data source: The Hydrogen Economy, M. Ball 2009 & Esprit Associates 2014

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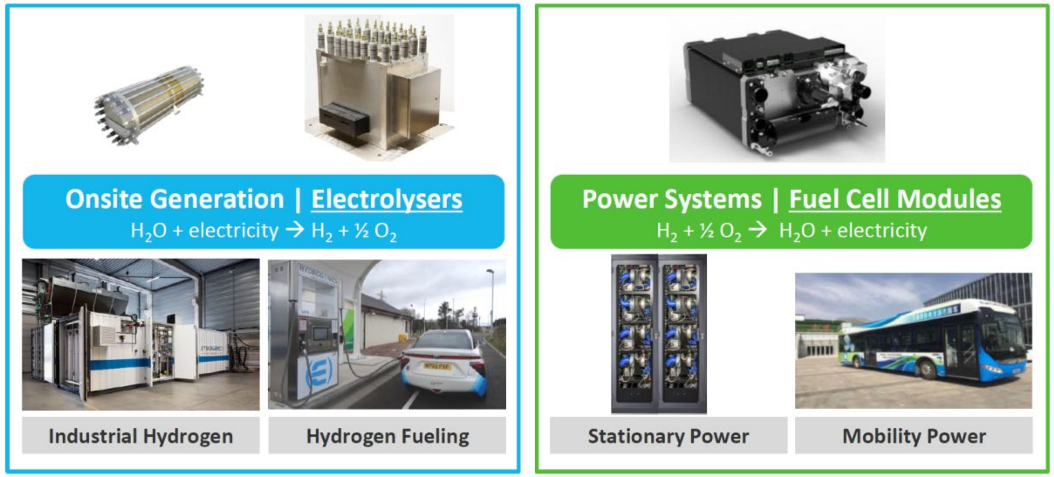
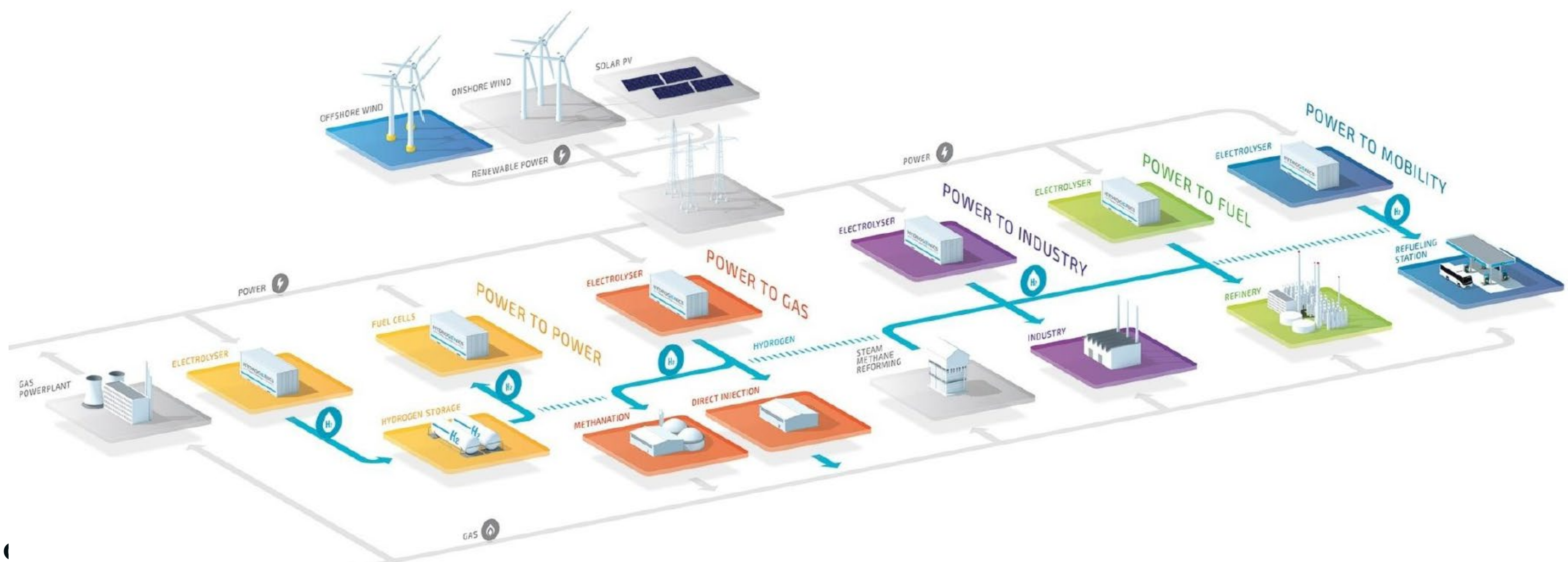
Applications of hydrogen





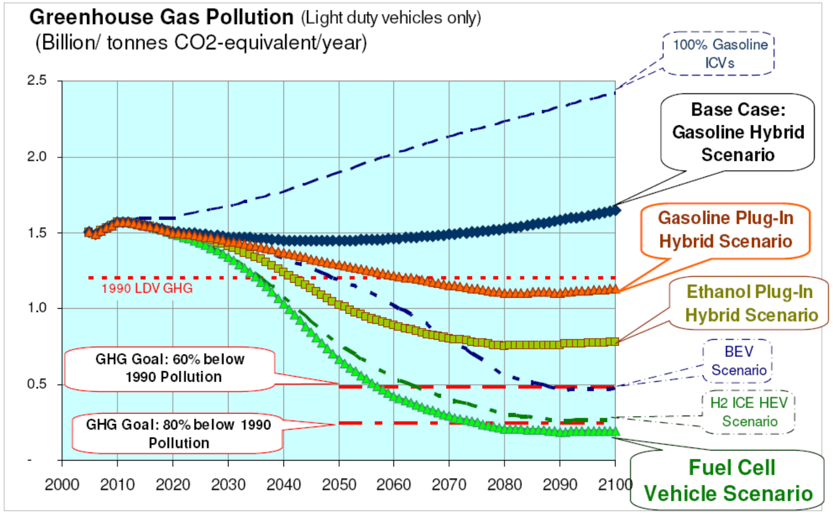
Hydrogen vehicles

- Hydrogen as fuel for green vehicles
- Range ~500 km/tank
- Quick refuelling (3-5 mins)

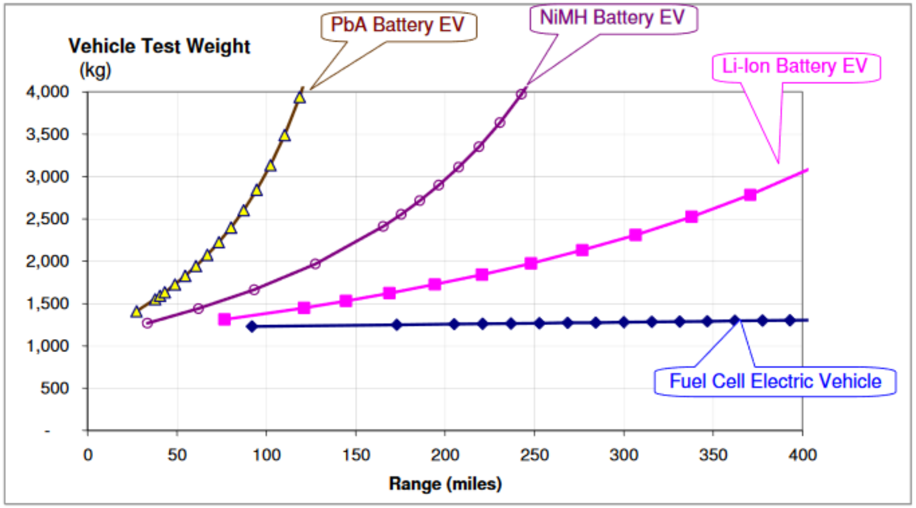
Toyota Mirai

Honda Clarity

Sold in US for $58,000 or $349/month lease



Projected greenhouse gas pollution for the U.S. light duty vehicles



Weight of electric vehicles as a function of vehicle range

Source: https://www1.eere.energy.gov/

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Hydrogen vehicles

'World's first' hydrogen-powered train enters into service

Anmar Frangoul

Published 5:29 AM ET Mon, 17 Sept 2018 | Updated 11:04 AM ET Mon, 24 Sept 2018

CNBC

https://www.cnbc.com/2018/09/17/worlds-first-hydrogen-powered-train-enters-into-service.html

Alstom | R Frampe

- 100 km route from Cuxhaven to Buxtehude
- Capacity: 160 passengers
- Top speed: 140 km/h
- Range: 1000 km/tank
- High capital cost but cheaper to run
- Another 14 hydrogen powered trains will be delivered in few years time.

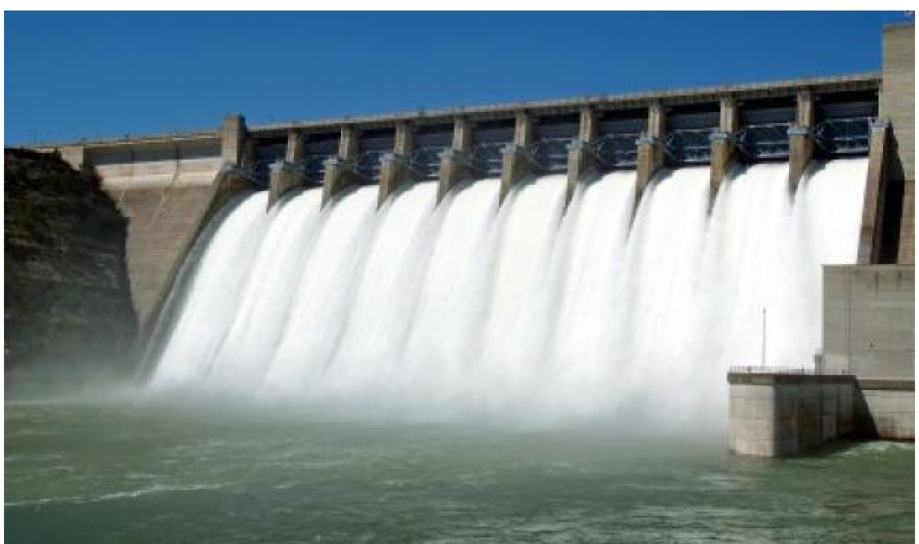
Hydrogen Bus in the UK

Sunline Transit H2 Bus in CA

Hydrogen Bus in Norway

Sarawak hydrogen production plant

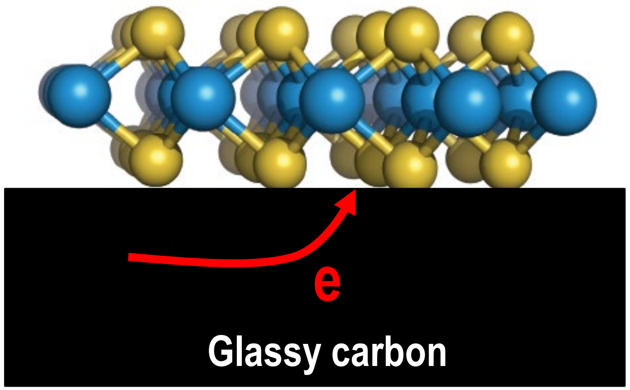
- Sarawak has abundant of water and hydroelectric power plant
- RM12 million of investment
- Opened May 2019
- Produces 130 kg of H_2 per day
- Five hydrogen vehicles: 3 buses & 2 cars
- Six 3-in-1 refueling stations by 2020



Basic principles in electrocatalysis

Step 1: Electron injection

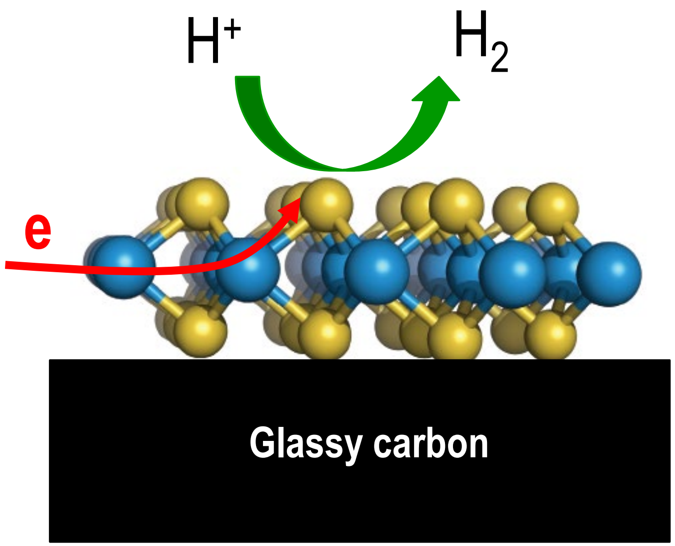
minimum charge transfer resistance, R_{CT}



Step 2: Electron transport to active site

Step 3: Reaction at the active site

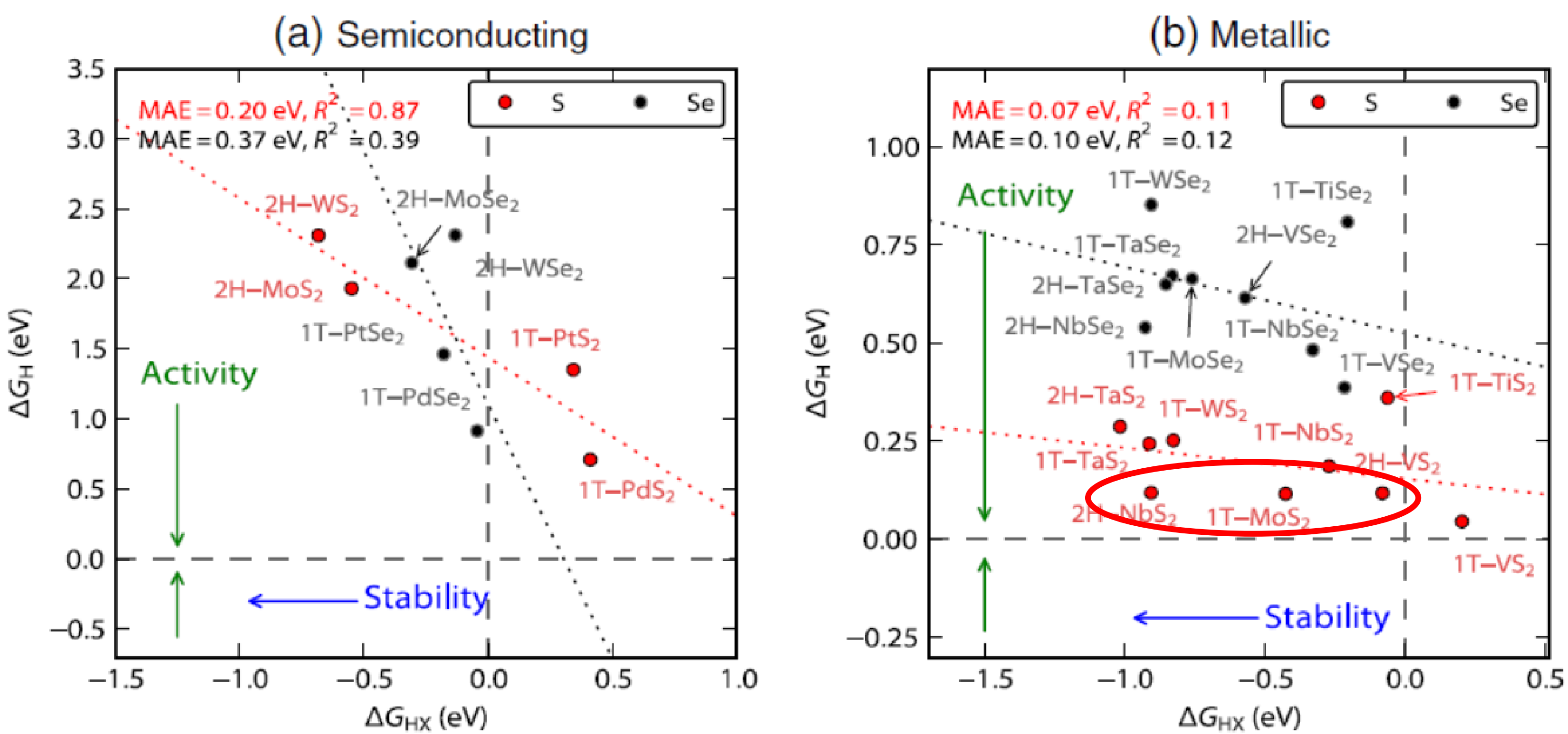
Interaction between catalyst and reactant should neither too weak nor too strong ($\Delta G_H \sim 0$ eV)



- $H^+ + e^- + * \rightarrow H^*$ (Volmer reaction)
- $2H^* \rightarrow H_2 + 2e^*$ (Tafel) or
  $H^* + e^- + H^+ \rightarrow H_2 + *$ (Heyrovsky)

Metallic 2D TMDs

- Interaction between catalyst and reactant should neither too weak nor too strong ($\Delta G_H \sim 0$ eV)
- Tsai *et al.* reported that the basal plane of metallic TM sulfides are the most active. Calculation based on ML TMDs *[Tsai et al., Surf. Sci. 640 133 (2015)]*

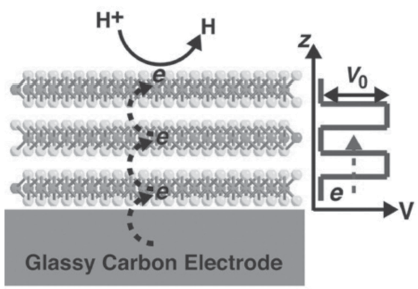


Hydrogen adsorption free energy for various TMDs

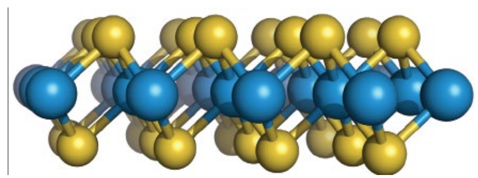
Improvement Strategies

Objectives: Low overpotential, low Tafel slope, high current density

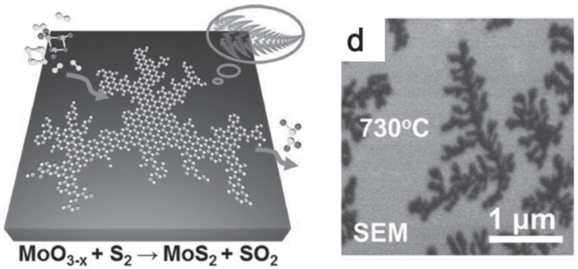
Electron transport



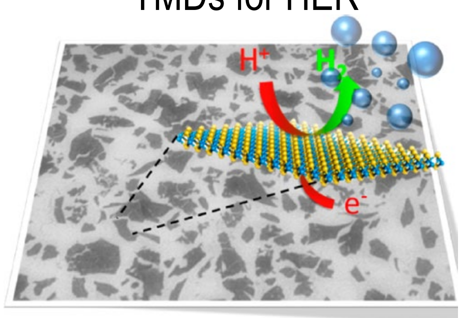
Metallic phase



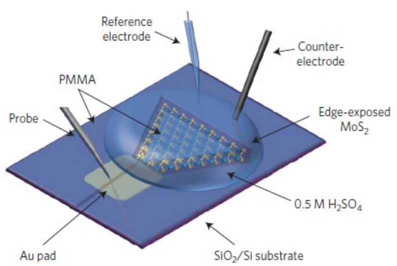
Increasing edges

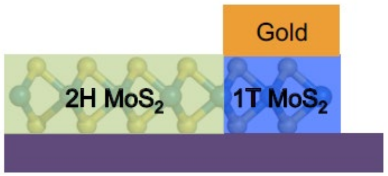


TMDs for HER

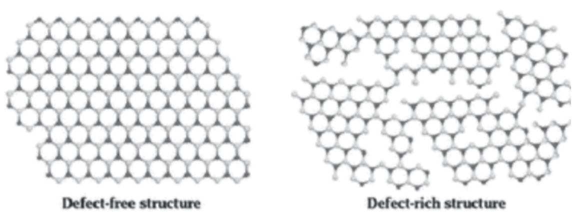


Coupling with substrate

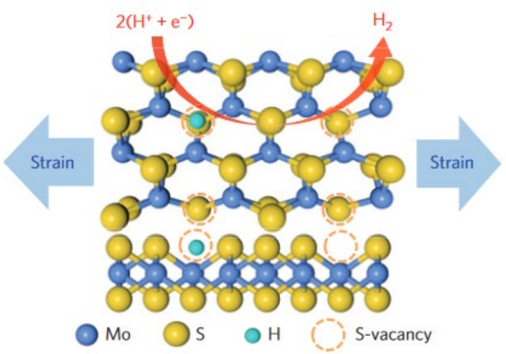




Defects



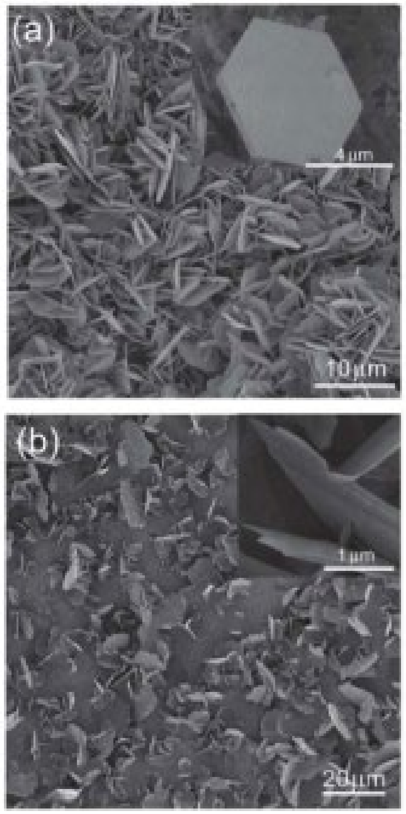
Strain



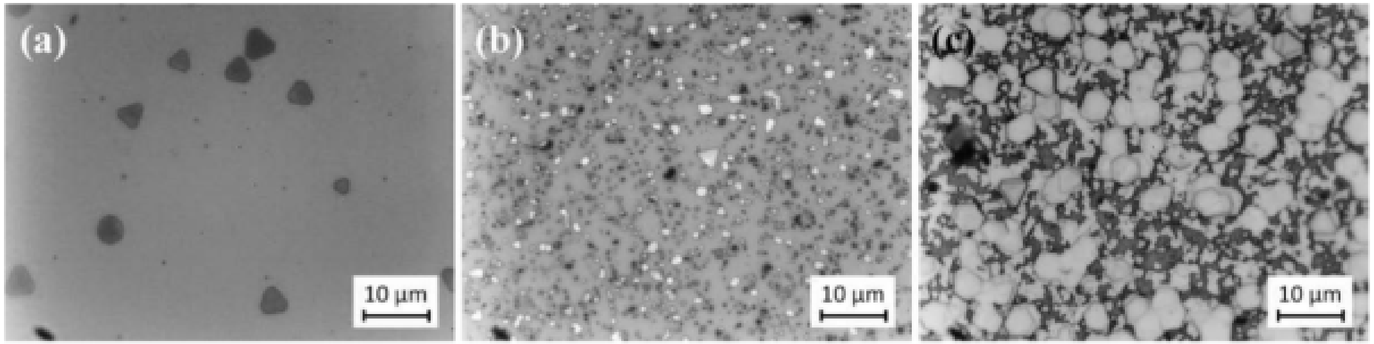
CVD of NbS_2

- Majority of previous works reported 3R-NbS_2 with thickness 20-500 nm
- Growth requires lots of sulfur, high temp. and high gas flow

Ref.	$NbCl_5$ (g)	S (g)	T_g (°C)	Growth time (mins)	Carrier gas (sccm)
Yanase et al, 2016	0.3	1.5	1000	30-120	ArH, 800-2000
Zhao et al, 2016	-	-	1050	10	Ar, 400
Das et al, 2015	-	8-10	850	30	Ar, 200
Ge et al, 2013	-	-	800	10	Ar, 200



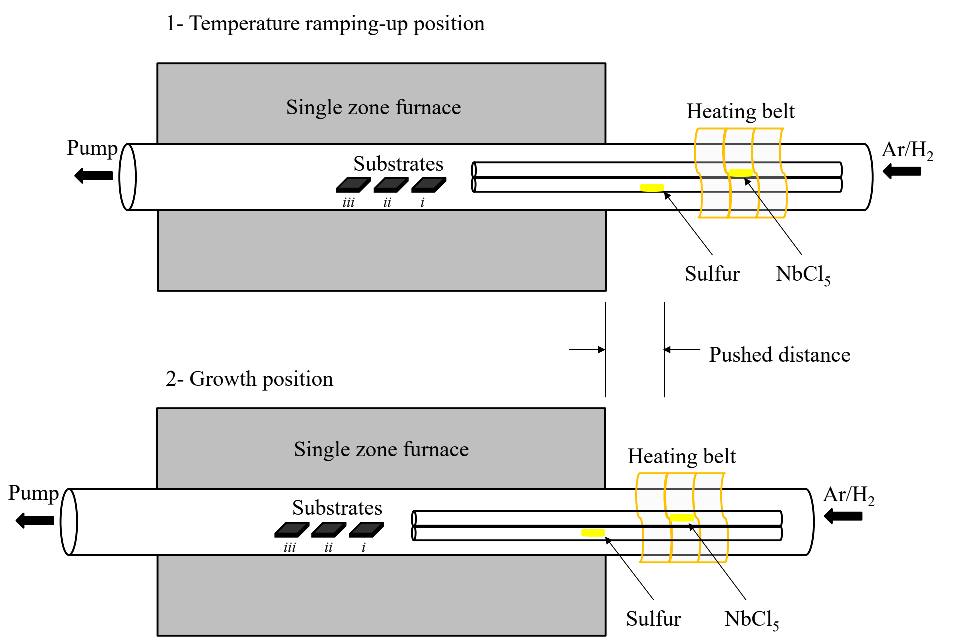
Ge et al, 2013



Yanase et al, 2016

CVD of NbS_2

- Growth conditions
  - Precursors: 40 – 60 mg of $NbCl_5$ and 140-200 mg of Sulfur
  - Substrate: SiO2/Si, glassy carbon
  - Substrate temp. / growth time : 1000 ^{o}C / 8-15 mins
- Heating belt is used to independently control the temp. of $NbCl_5$.
- Small quartz tubes are also used to avoid cross contamination.



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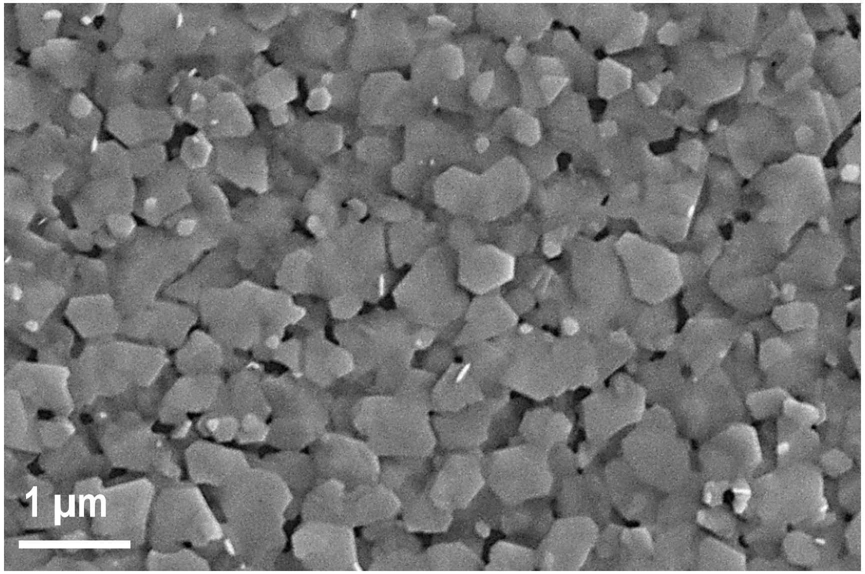
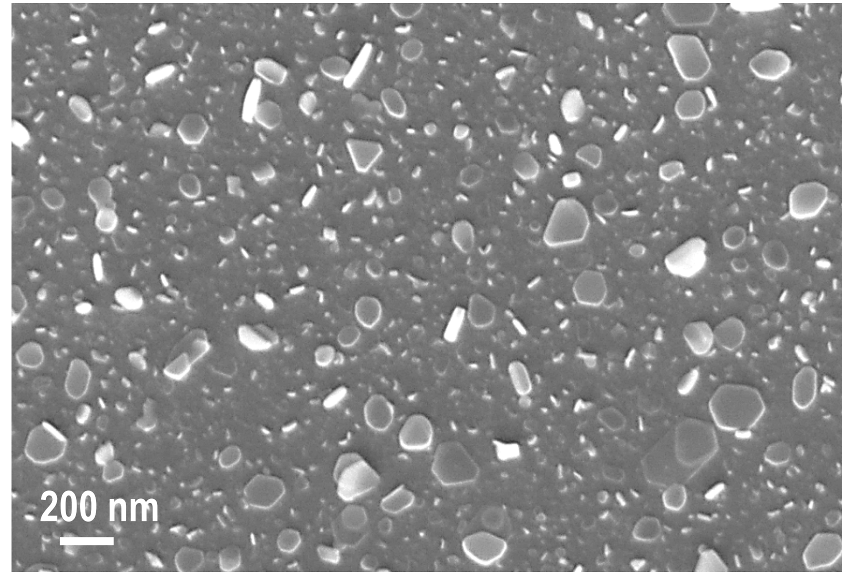
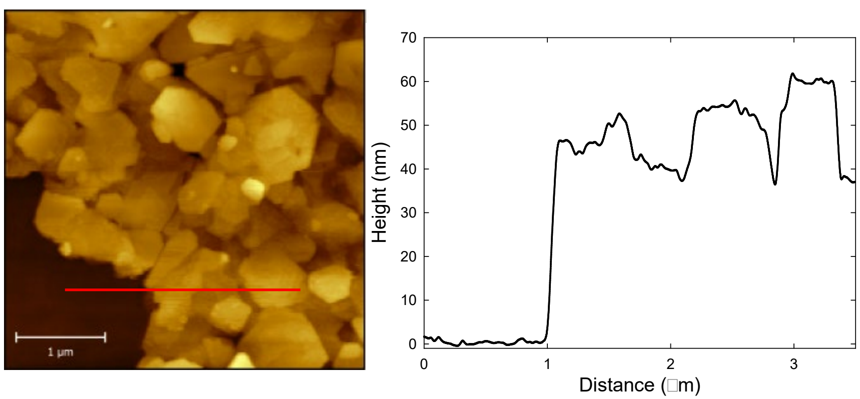
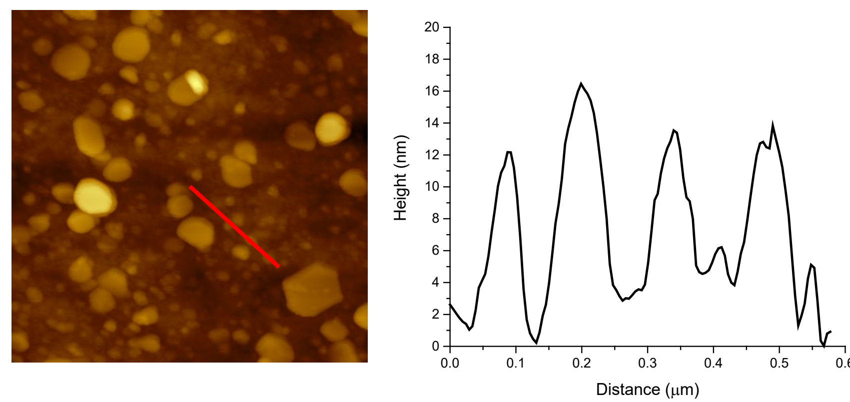
CVD of NbS_2









40 mg NbCl5, 15 mins:
film with thickness ~50 nm

40 mg, 8 mins growth: small individual flakes with lateral dimension ~200 nm & thickness ~15 nm

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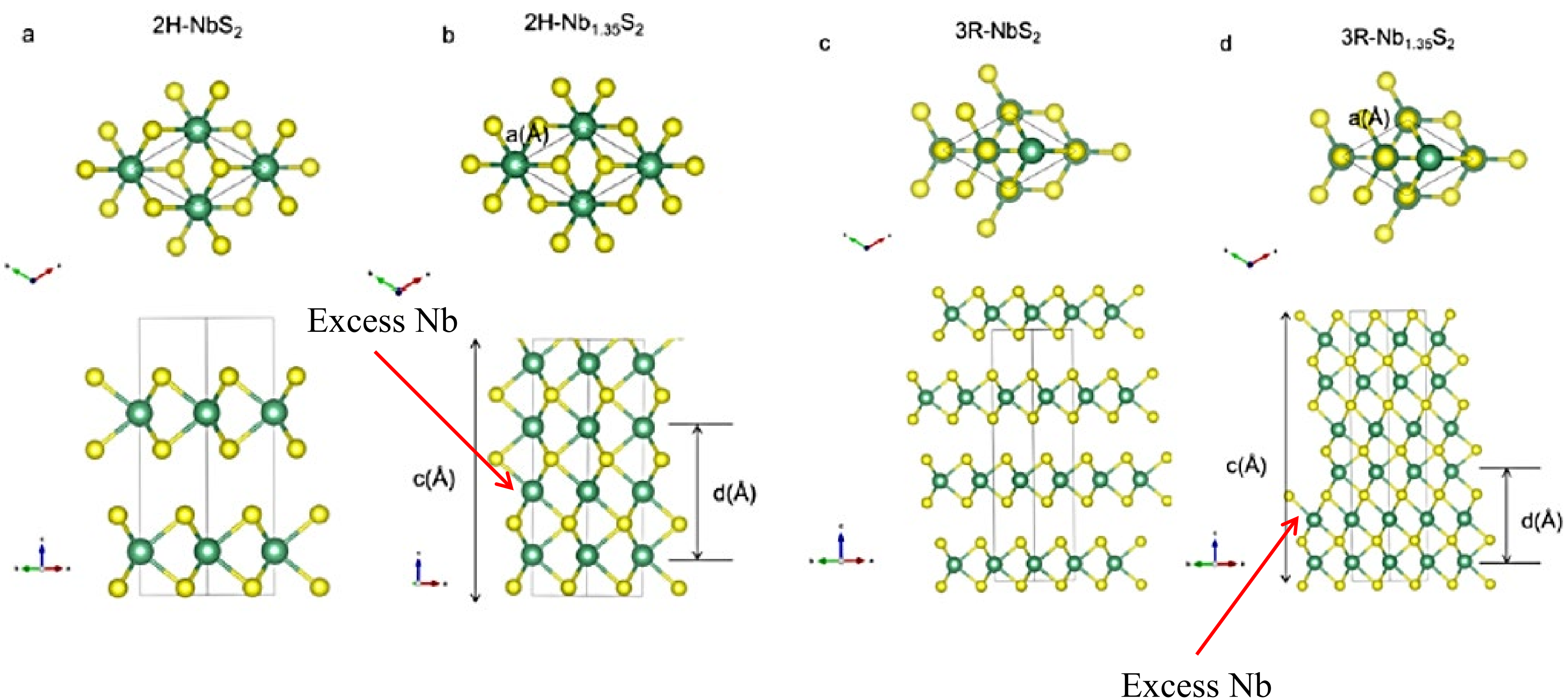
Nb Interstitials in NbS_2

- Nb interstitials may presence in between the layers



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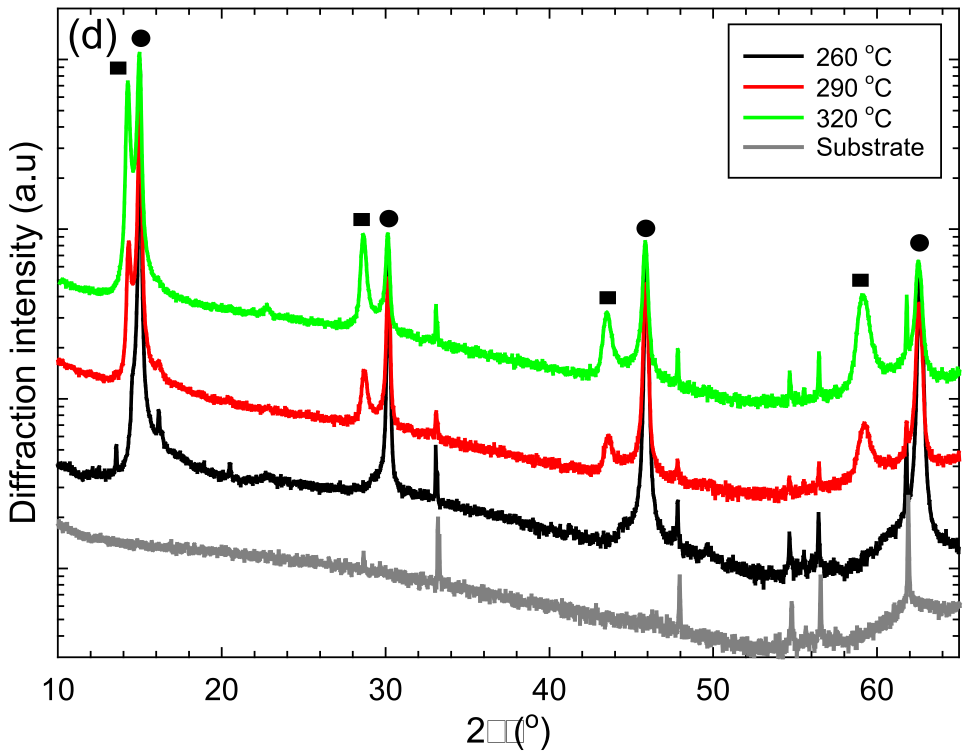
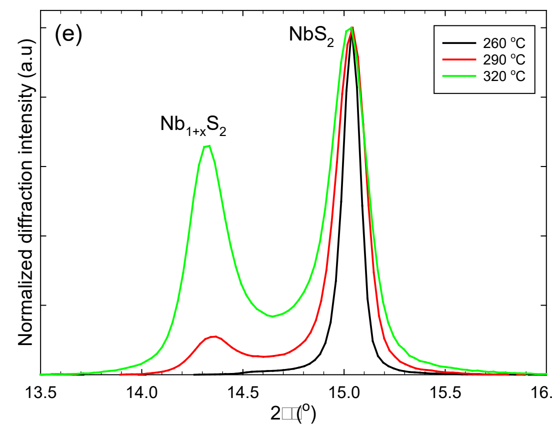
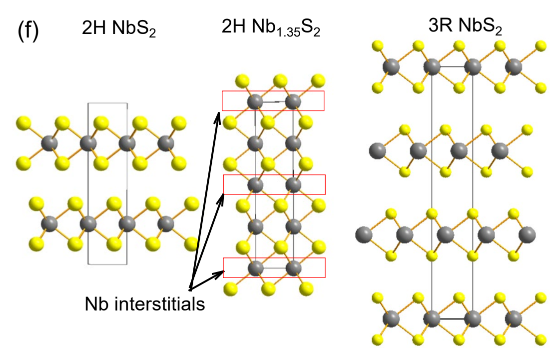
Nb Interstitials in thin NbS_2

- NbS_2 samples were grown with different $NbCl_5$ temperatures (260-320 ^oC)
- Peaks ■ can be fitted with 1 possibility: Hexagonal $Nb_{1.35}S_2$, (P63/mmc): PDF#97-004-3699



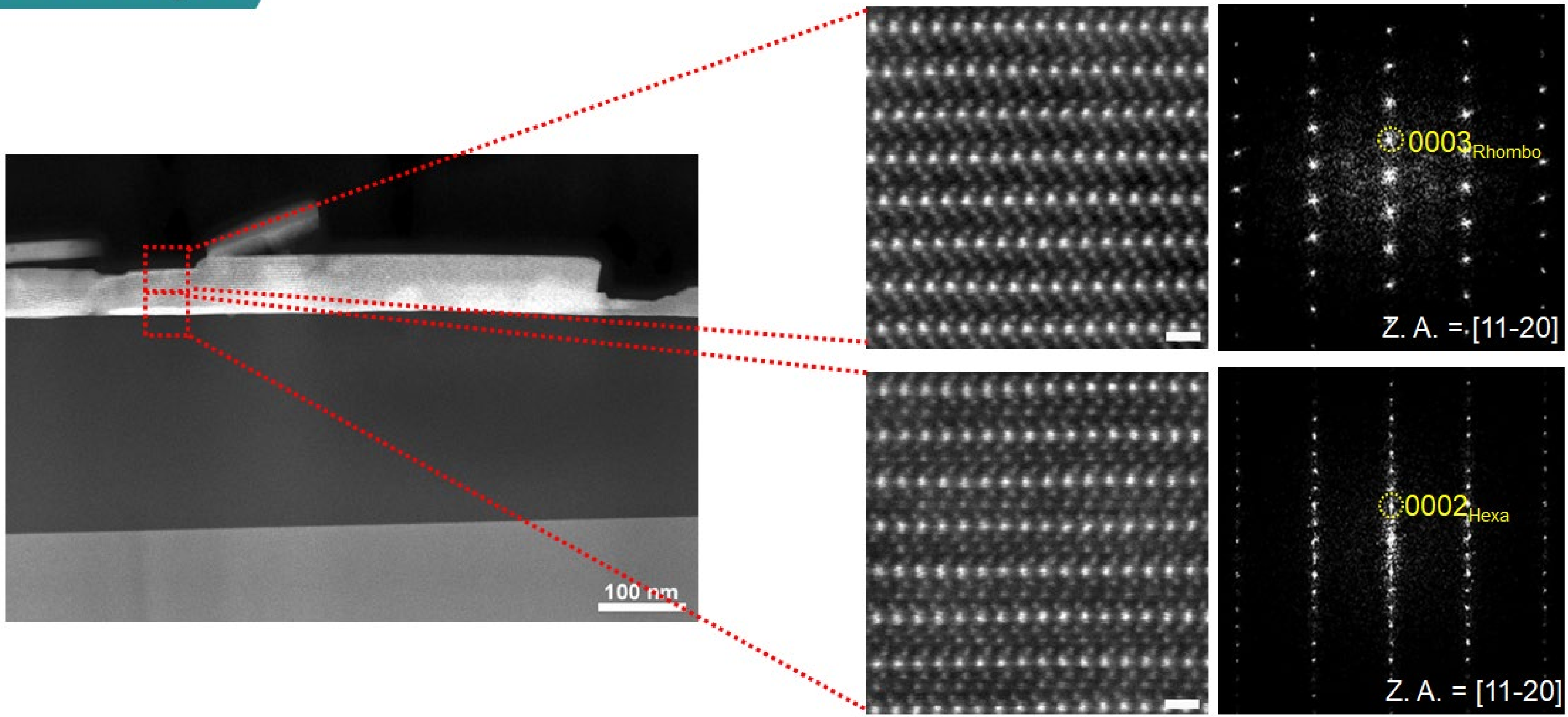




Nb Interstitials in thin NbS_2

- HR Annular Dark Field (ADF) STEM Images were taken with Titan microscope at 200 kV

STEM images



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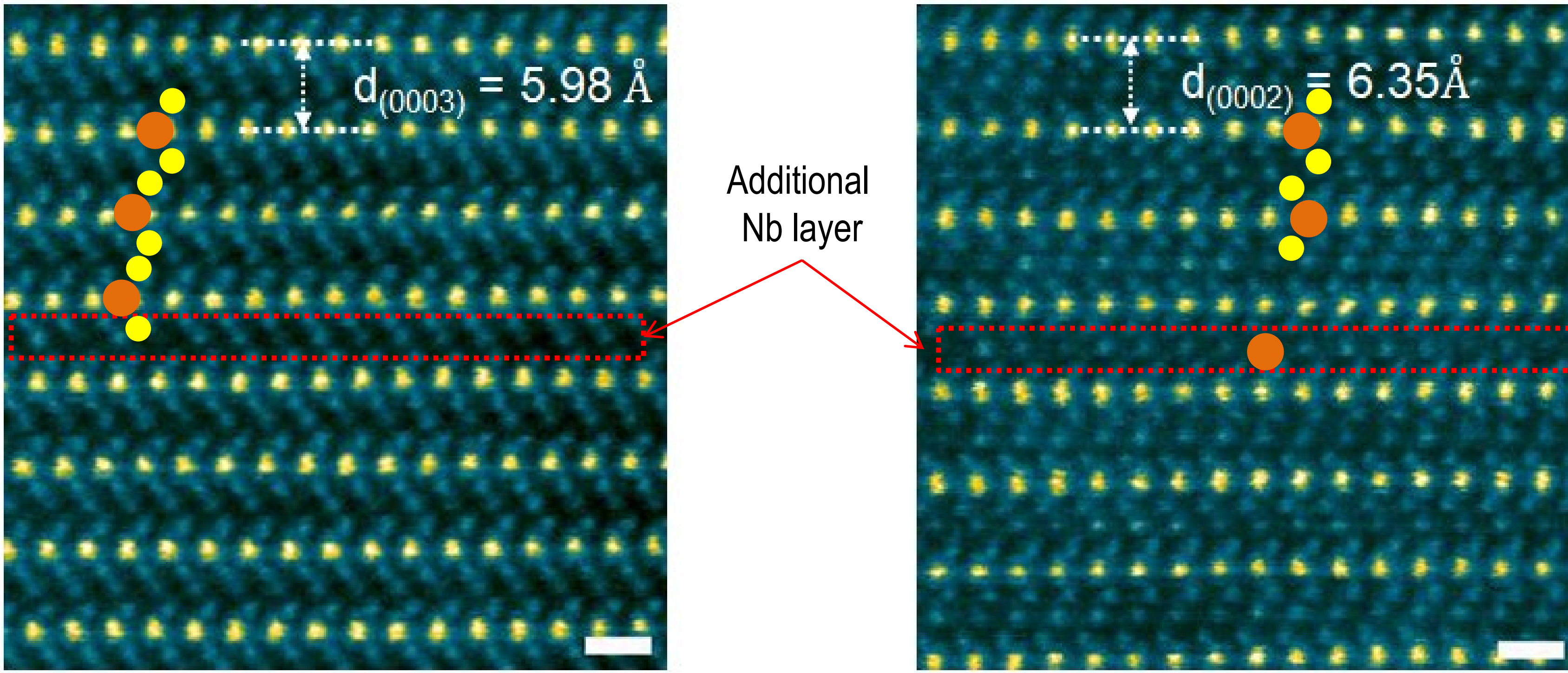
Nb Interstitials in thin NbS_2

- We can observe additional Nb layers in the structure



NbS_2 Rhombohedral		$Nb_{1.35}S_2$ Hexagonal
a=3.33Å, c=17.81Å	*Theoretical value*	a=3.31Å, c=12.6Å

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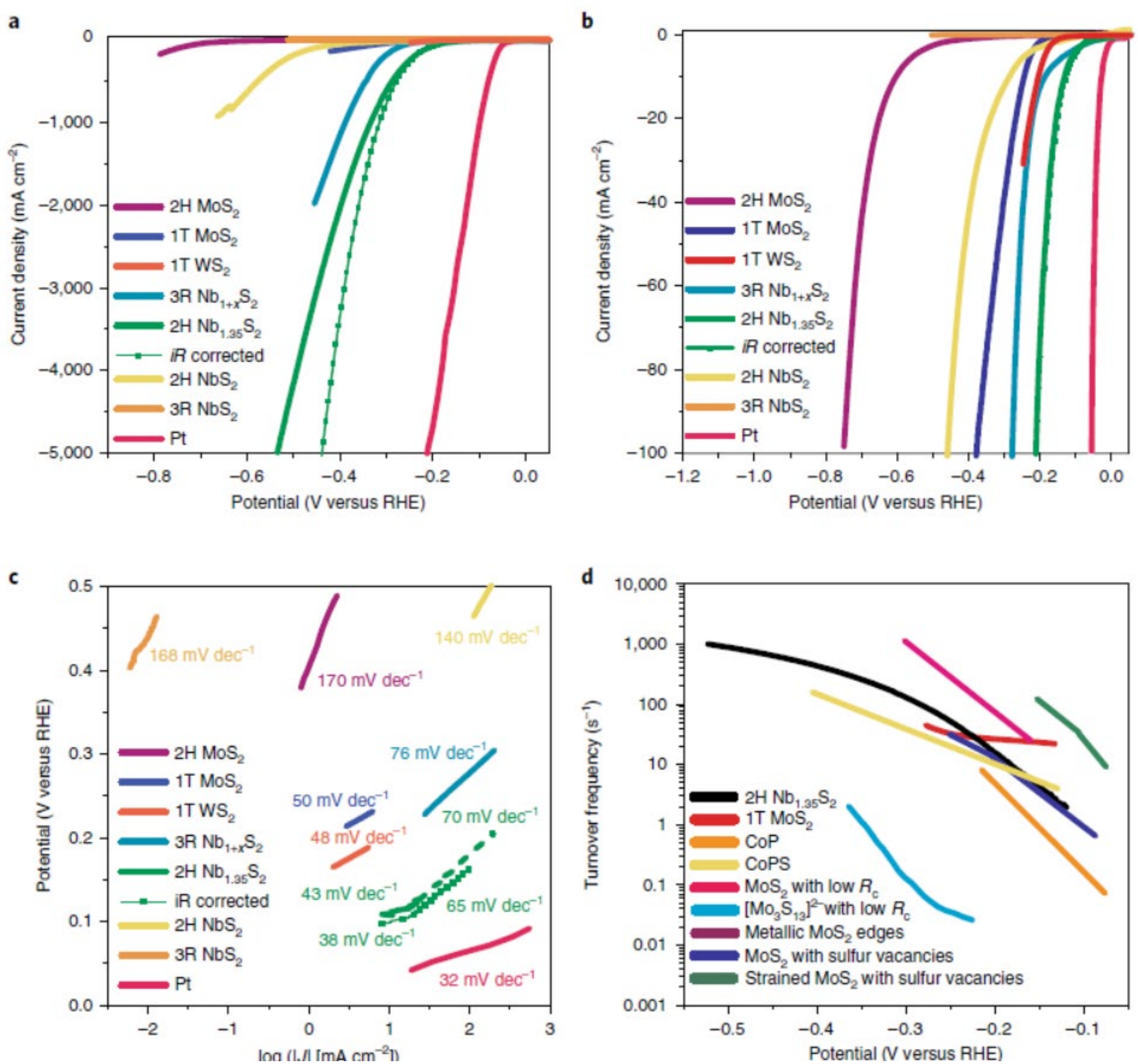
HER with exceptionally large current density



Polarization curves for various TMDs and Pt measured in 0.5M H_2SO_4 (scan rate of 5 mVs^{-1})

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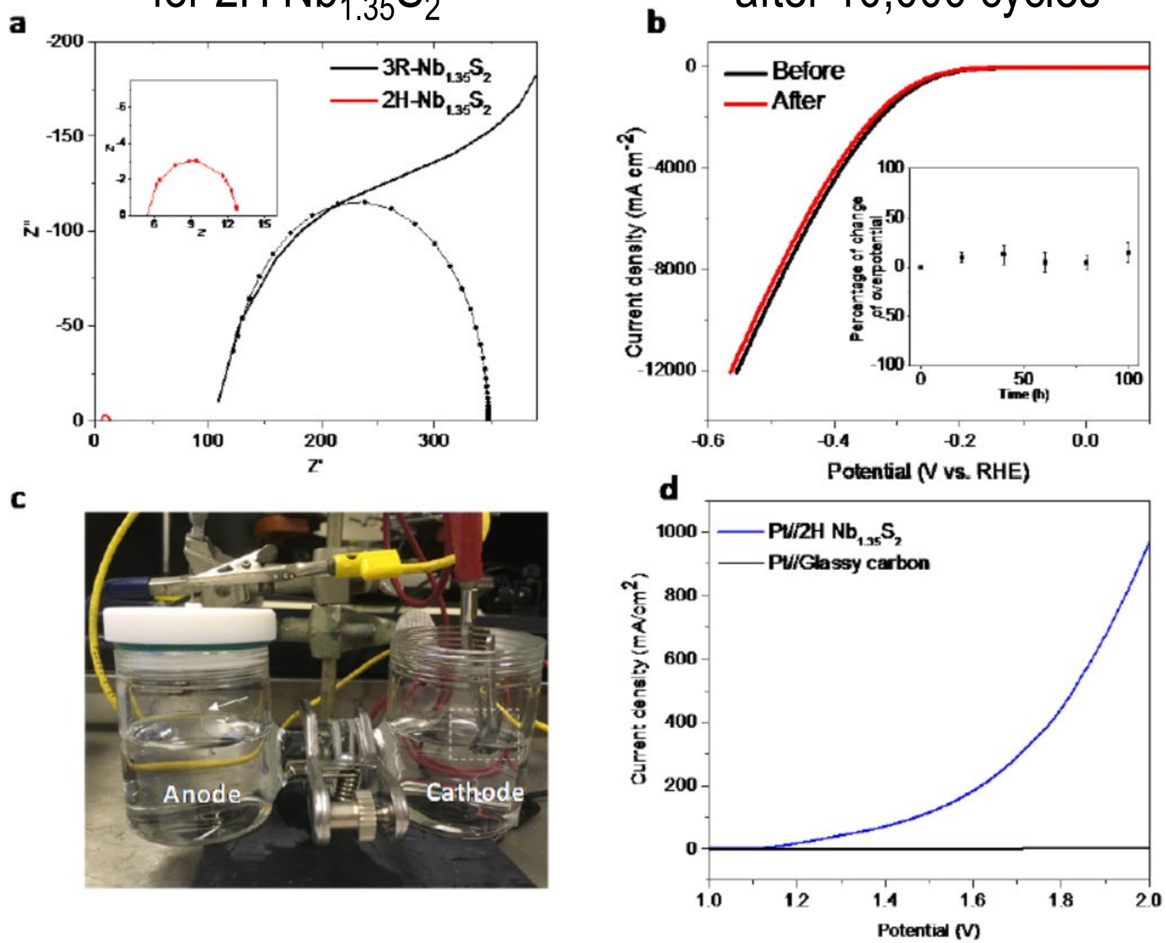
Electrolyzer with high current density

EIS measurements for 2H $Nb_{1.35}S_2$

Stability measurements after 10,000 cycles

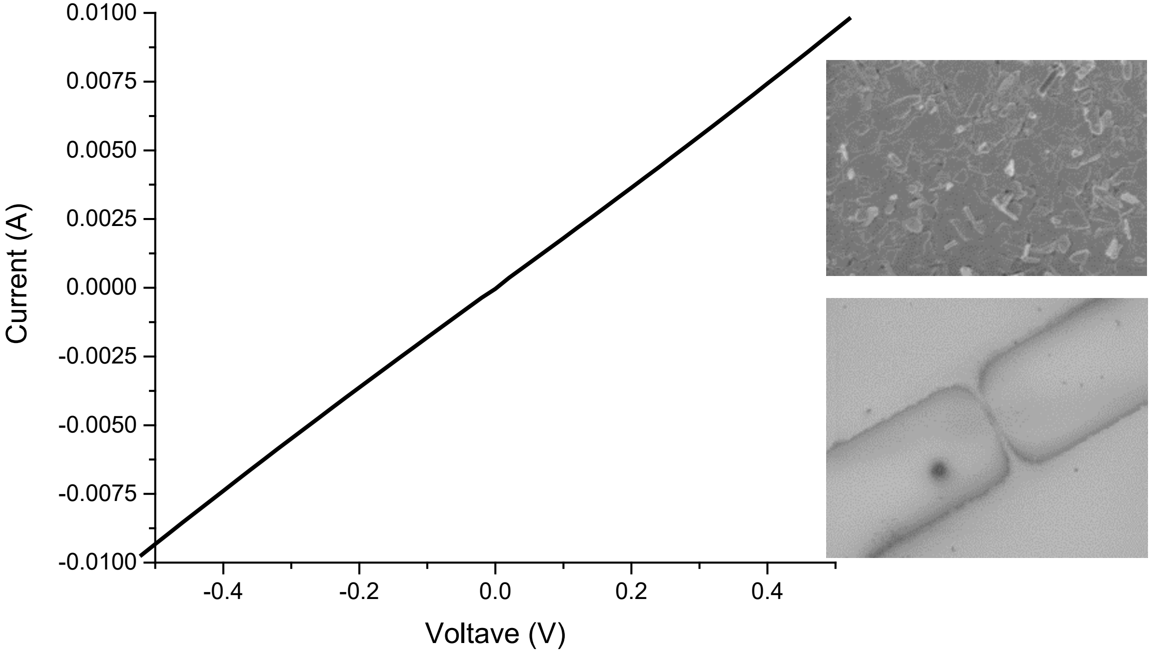


Proof of concept 2-electrode electrolyzer

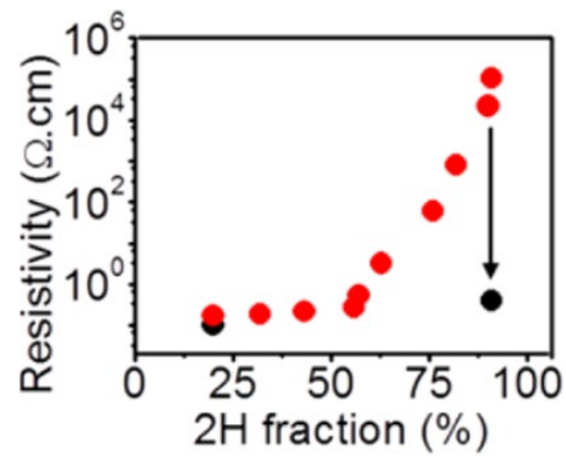
Polarization curve of water electrolysis

Electrical Results

- All devices show linear I-V curves suggesting ohmic contact with metallic channel
- Resistivity (from 15 devices) : 2-6 x 10^{-3} Ωcm
- Large current density : 2-6 x 10^{4} A/cm^{2} at 0.5 V



Resistivity of 1T and 2H MoS2

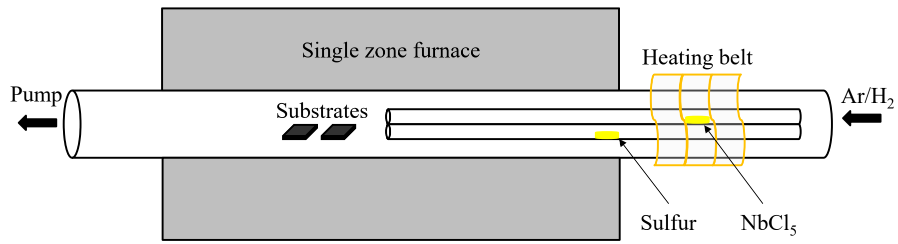


Voiry et al, Nano Lett 13 (2013) 6222

Key results

The reported **niobium disulfide** ($Nb_{1.35}S_2$) catalyst:

- **Low cost**
- **Performance on-par with platinum**



Ref.: alfa aesar & sigma aldrich

chemical vapor deposition (CVD) at high temperature and low pressure

Platinum

~RM 1000/gram

vs

Niobium Chloride

~RM 10/gram

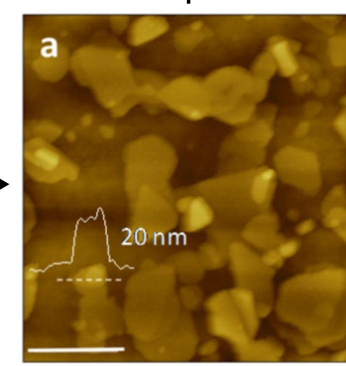
+

Sulfur

~RM 0.50/gram

→

Niobium disulphide



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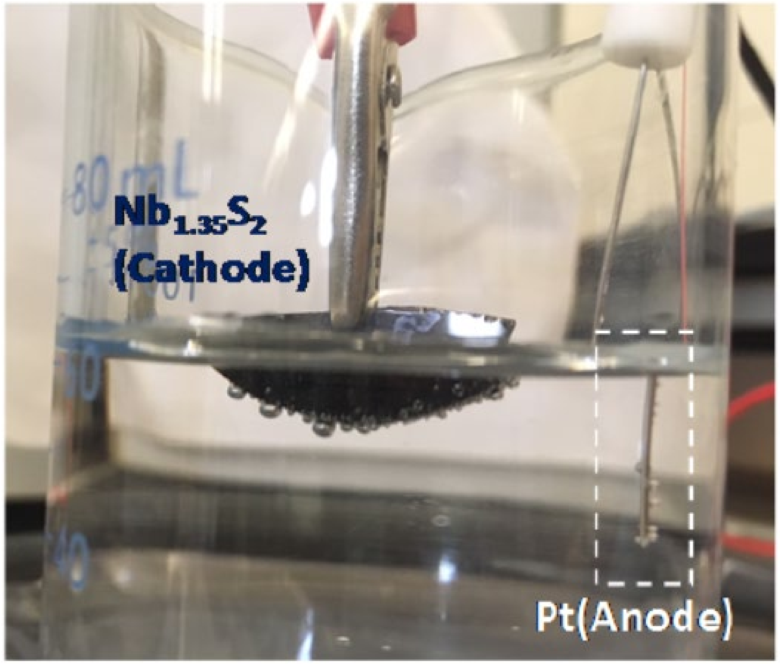
Key results

Hydrogen evolution comparison:

- Most of 2D based catalyst: 10 – 100 $mAcm^{-2}$
- Platinum based catalyst >1000 $mAcm^{-2}$
- Our work (niobium disulfide) >5000 $mAcm^{-2}$
- Highly stable (measurements up to 10,000 cycles)



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More details

- Full article can be accessed at:

https://www.nature.com/articles/s41563-019-0463-8

nature materials

LETTERS

https://doi.org/10.1038/s41563-019-0463-8

Ultrahigh-current-density niobium disulfide catalysts for hydrogen evolution

Jieun Yang[1,10], Abdul Rahman Mohmad[2,10], Yan Wang[1], Raymond Fullon[1], Xiuju Song[1,3], Fang Zhao[4], Ibrahim Bozkurt[1], Mathias Augustin[5], Elton J. G. Santos[5*], Hyeon Suk Shin[6], Wenjing Zhang[3], Damien Voiry[7], Hu Young Jeong[8*] and Manish Chhowalla[1,3,9*]

Metallic transition metal dichalcogenides (TMDs)[1–8] are good catalysts for the hydrogen evolution reaction (HER). The overpotential and Tafel slope values of metallic phases

density. Thus, a fine balance must be achieved between reducing the thickness of catalysts and maintaining metallic nature of 2D materials to maximize catalytic performance.

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Outline

- Research journey
  - PhD study at University of Sheffield, UK
  - Transition from PhD to academia
  - Postdoctoral experience at Rutgers University, US
- Our findings & publishing in Nature Materials
  - Application and demands for hydrogen
  - 2D Transition Metal Dichalcogenides (TMDs) catalyst for hydrogen evolution
  - Key results
- Work Life Balance

Take care of yourself

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Do charity. Help others

Relief mission to Gaza in 2012

Flood relief mission in Kuantan

Take a break

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Summary

Recipe for excellence

- Desire for excellence
- Willingness
- Hardwork

- Strategy (3 Rs)
- Discipline
- Attention to details
- Resources

- Tawakkal & prayer

Thank you for your attention. Any questions?

Contact details:
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"There's a lot of art in science. It's not just equations and formulas"
Alfred Cho