Charles Hatchett Webinar, 2020

Ultrahigh current density niobium disulfide catalysts for hydrogen evolution

Jieun Yang, Abdul Rahman Mohmad, Yan Wang, Raymond Fullon, Xiuju Song, Fang Zhao, Ibrahim Bozkurt, Mathias Augustin, Elton J. G. Santos, Hyeon Suk Shin, Wenjing Zhang, Damien Voiry, Hu Young Jeong, **Manish Chhowalla**

Materials Science & Metallurgy

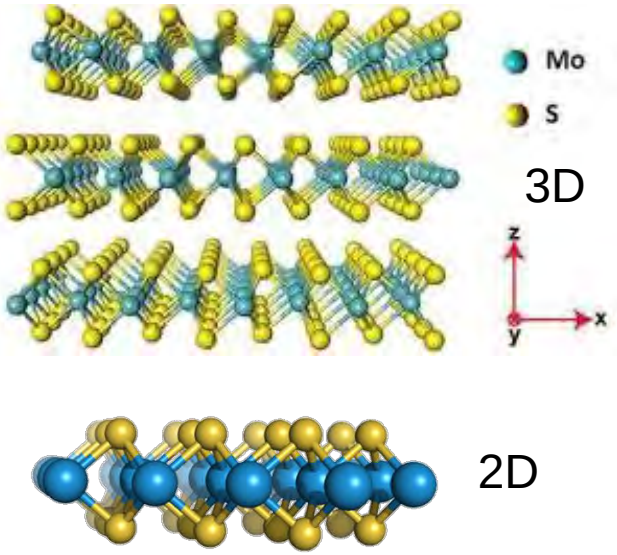
HENRY ROYCE INSTITUTE
UK NATIONAL INSTITUTE FOR ADVANCED MATERIALS
ROYCE.AC.UK

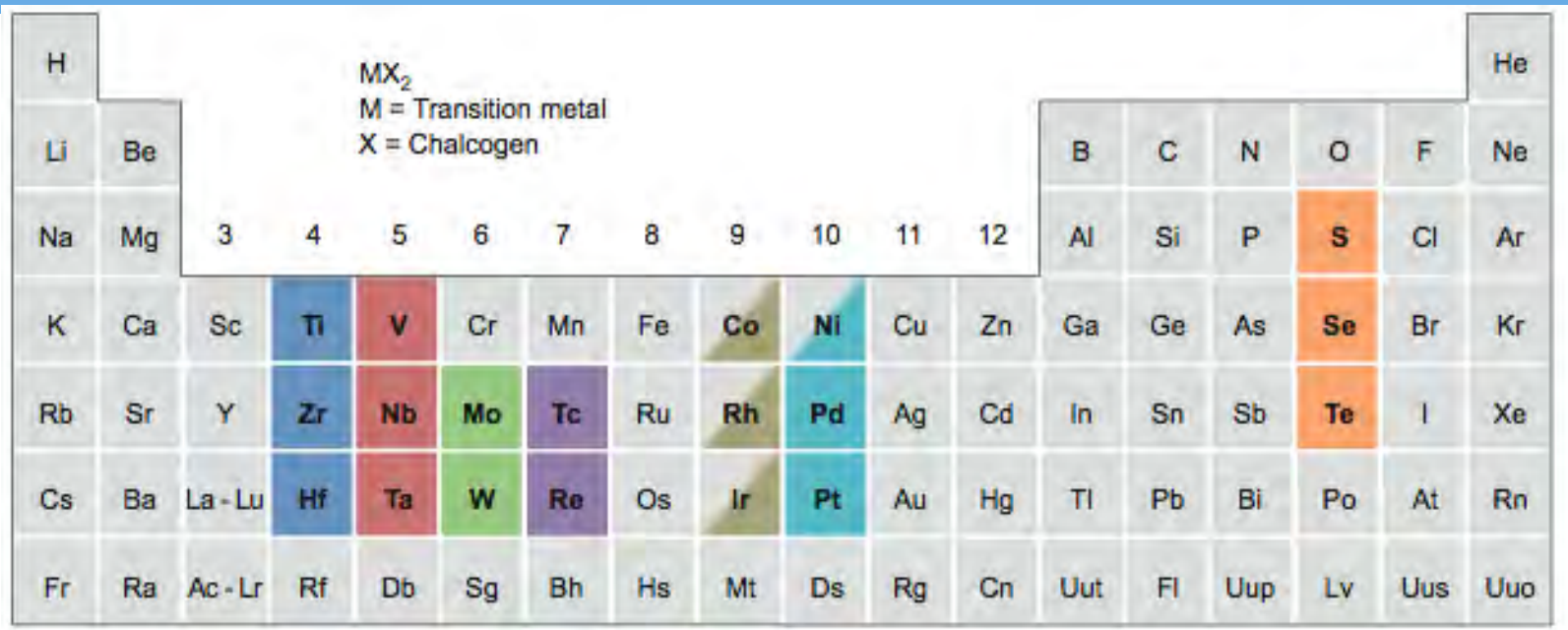
@chhowalla
@chhowallaL

UNIVERSITY OF CAMBRIDGE

Email: mc209@cam.ac.uk

Transition metal dichalcogenide 2D semiconductors



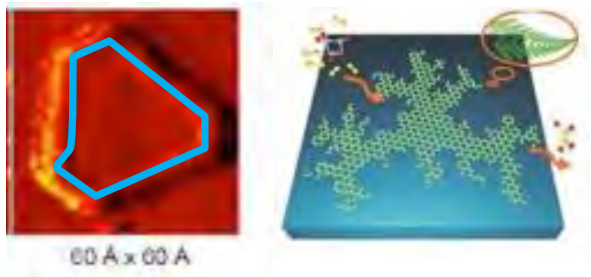


1T	d^0	Ti, Zr, Hf	S_2, Se_2, Te_2	Semiconducting (Eg = 0.2~2 eV), diamagnetic
2H or 1T	d^1	V, Nb, Ta	S_2, Se_2, Te_2	Narrow band metals (10^{-4} Ω.cm) or semimetals, superconducting
Mostly 2H	d^2	Cr, Mo, W	S_2, Se_2, Te_2	Semiconducting (Eg = 1.5 eV), diamagnetic
Distorted 1T	d^3	Mn, Tc, Re	S_2, Se_2, Te_2	Antiferromagnetic or diamagnetic, small gap semiconductors

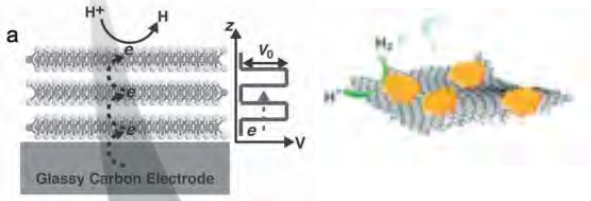
Chhowalla, Nature Chem. , 2013

2D materials as catalysts for hydrogen evolution reaction (HER)

Increasing edges

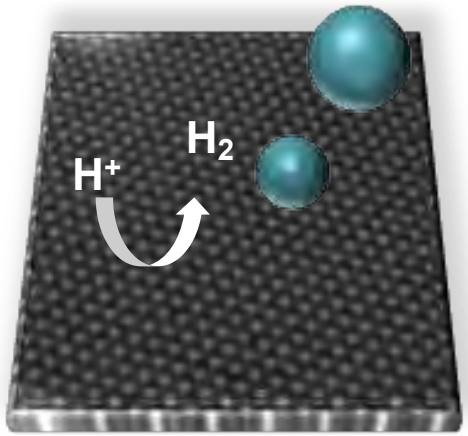


Electron transport

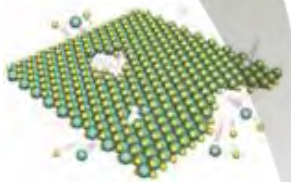


Synthesis of metallic TMD
-Challenging

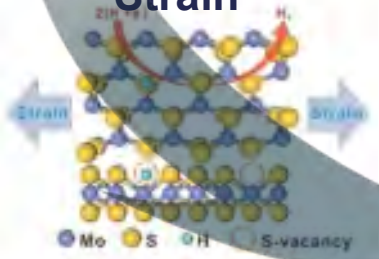
TMD for HER



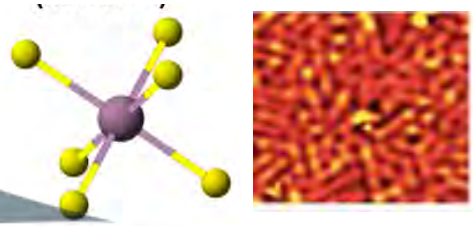
Defects



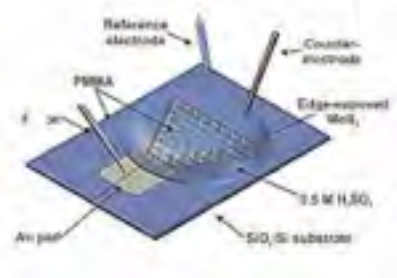
Strain



Metallic phase

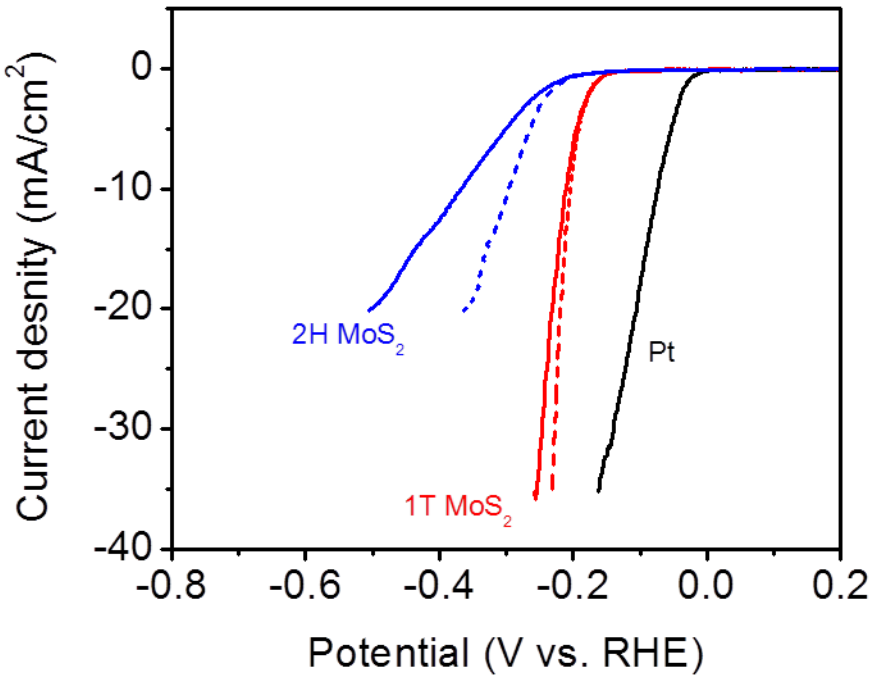


Coupling with substrate

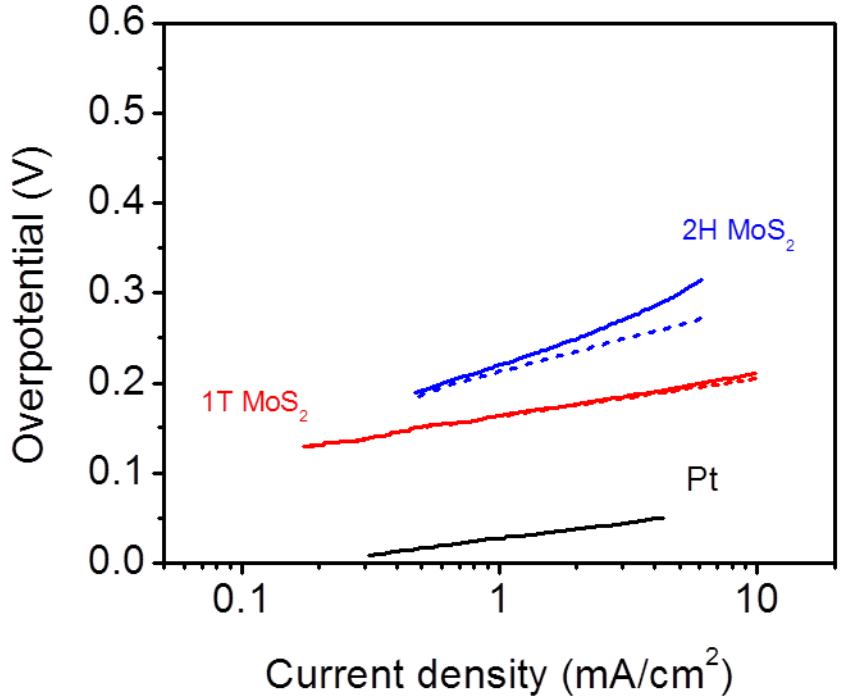


HER with Metallic 1T Phase MoS_2

Polarization curves: $2H^+ + 2e^- = H_2$



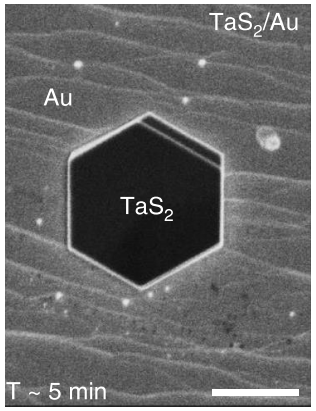
Tafel slope

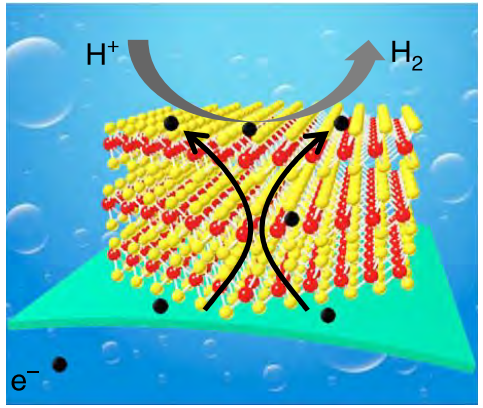


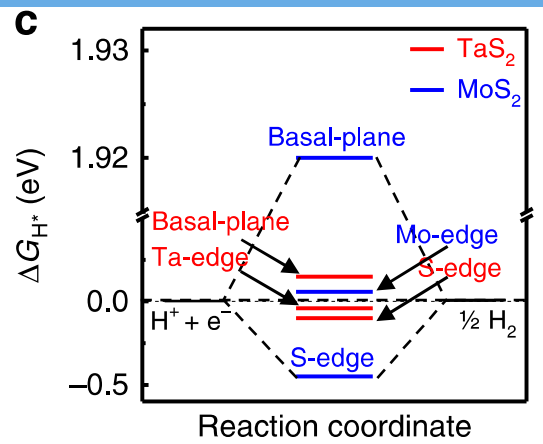
	1T-WS_2	**1T-MoS_2**
Overpot.	80 mV	**150 mV**
Tafel slope	~ 60 mv/dec	**~ 40 mV/dec**

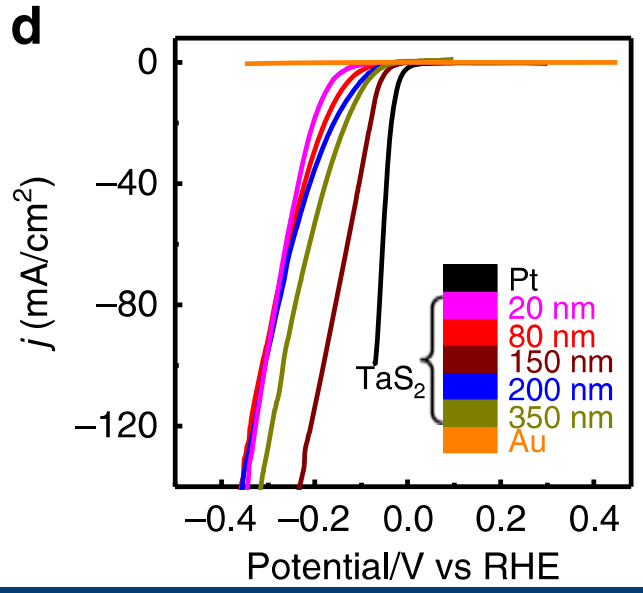
Metallic 2D TMDs as catalysts for HER

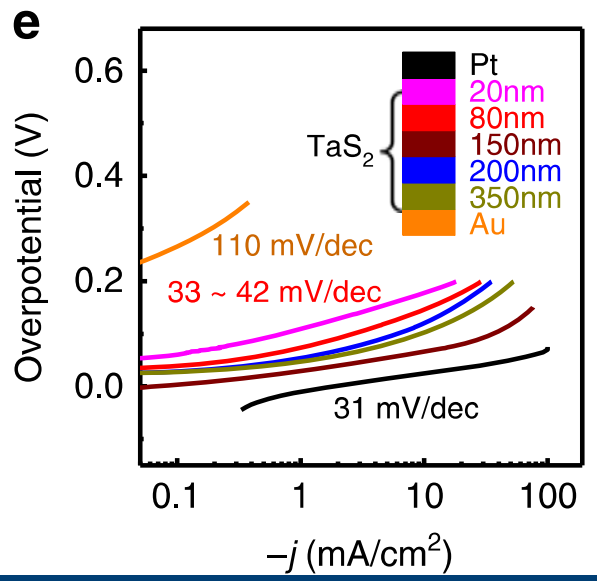
TaS_2 for HER from Yanfeng Zhang Group at Peking U (Nature Comm. 2017, 8, 958)

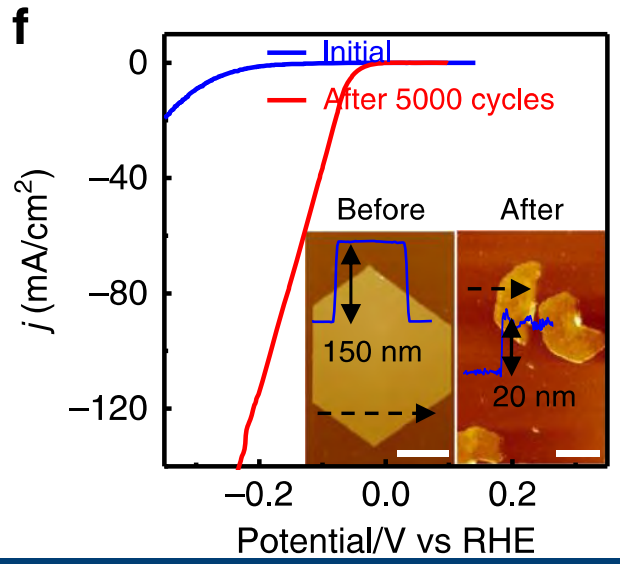








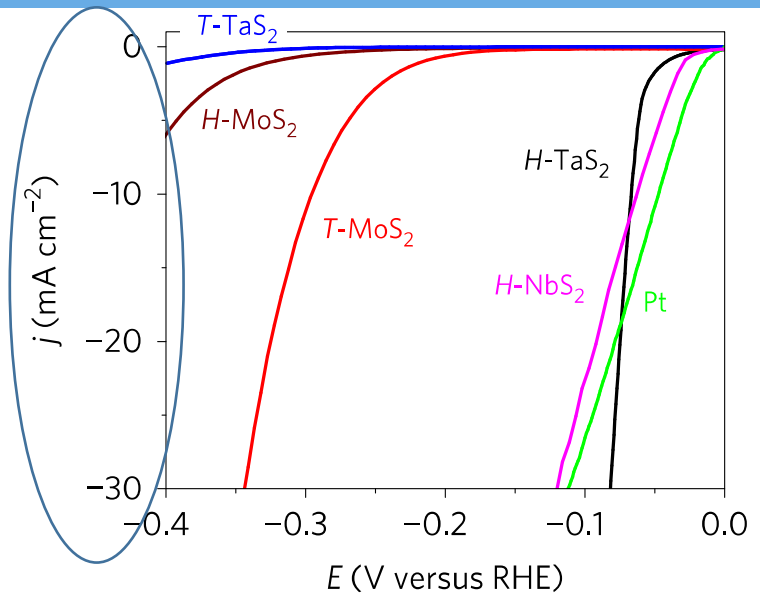


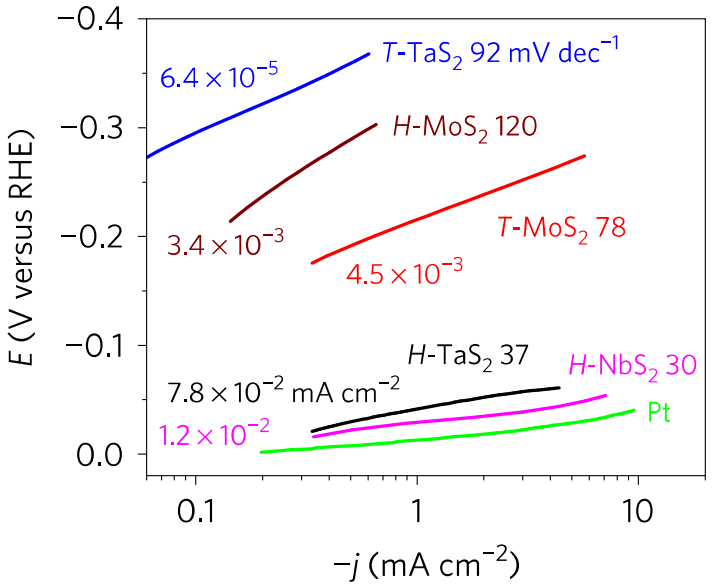


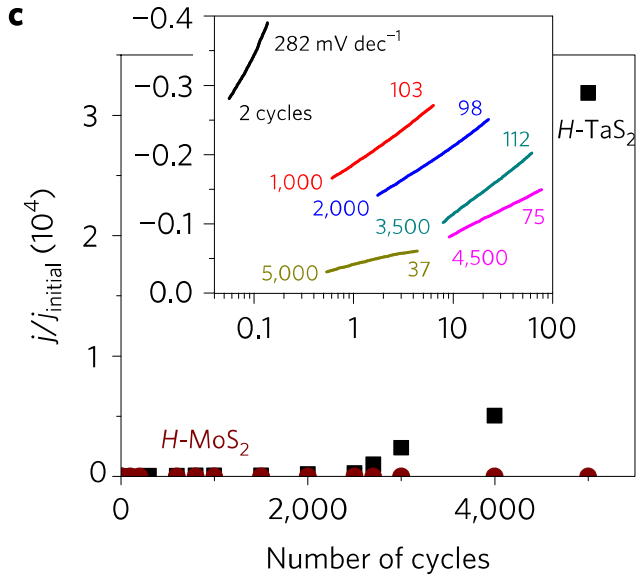
Metallic 2D TMDs as catalysts for HER

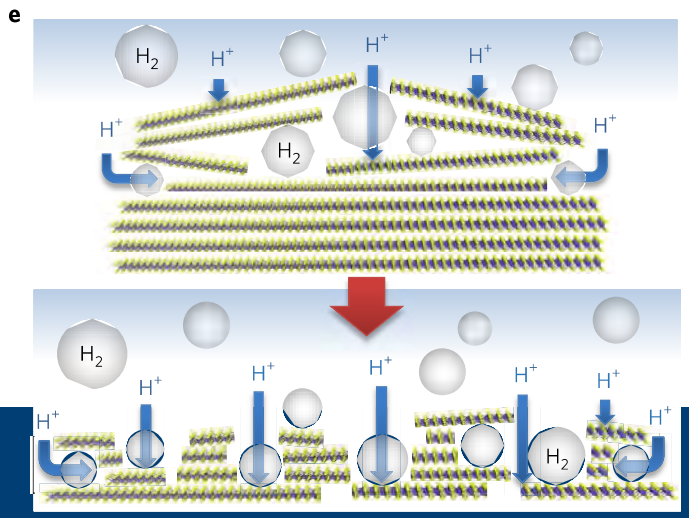
NbS_2 for HER from Yakobson Group at Rice U (Nature energy 2017, 2, 17127)

Very low current densities





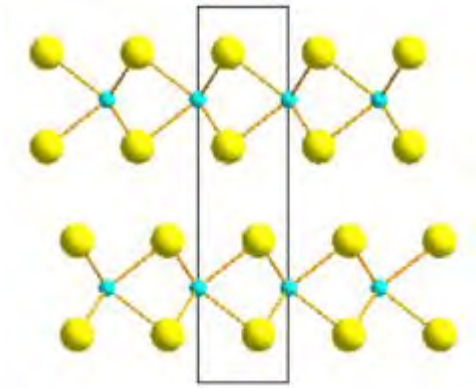




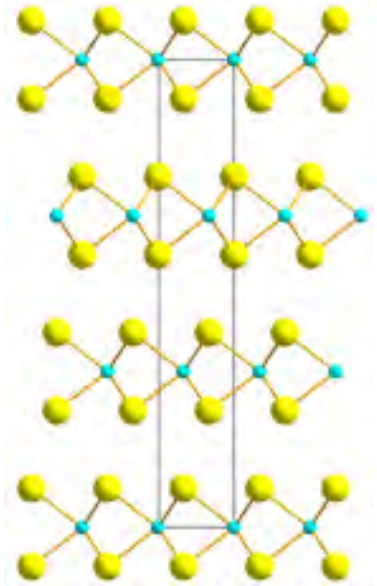
$Nb_{1.35}S_2$

Phases of NbS_2:

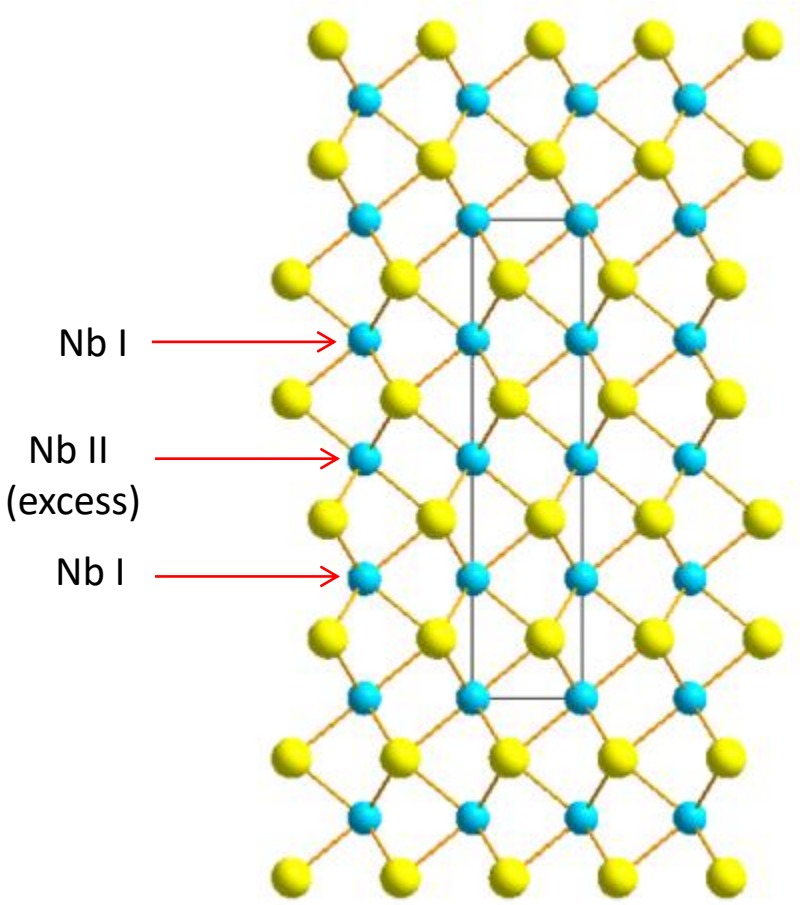
2H

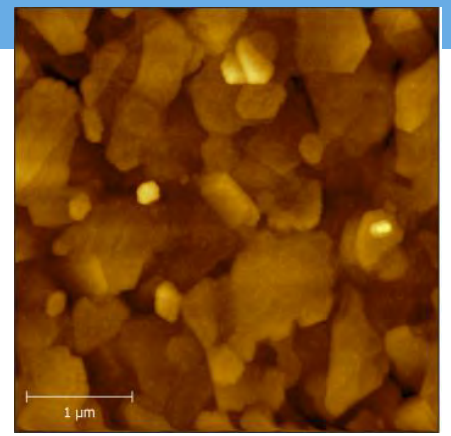


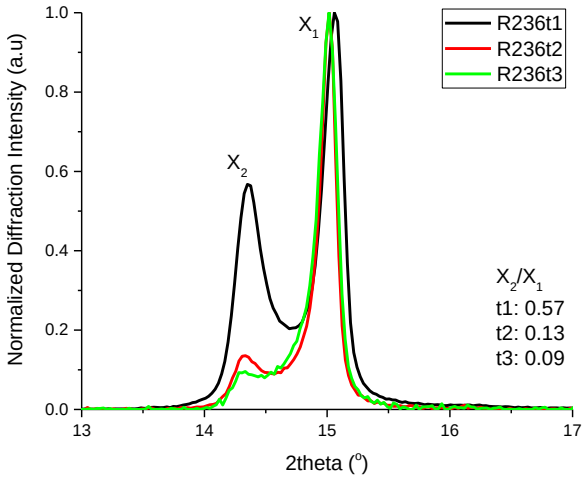
3R



$Nb_{1.35}S_2$

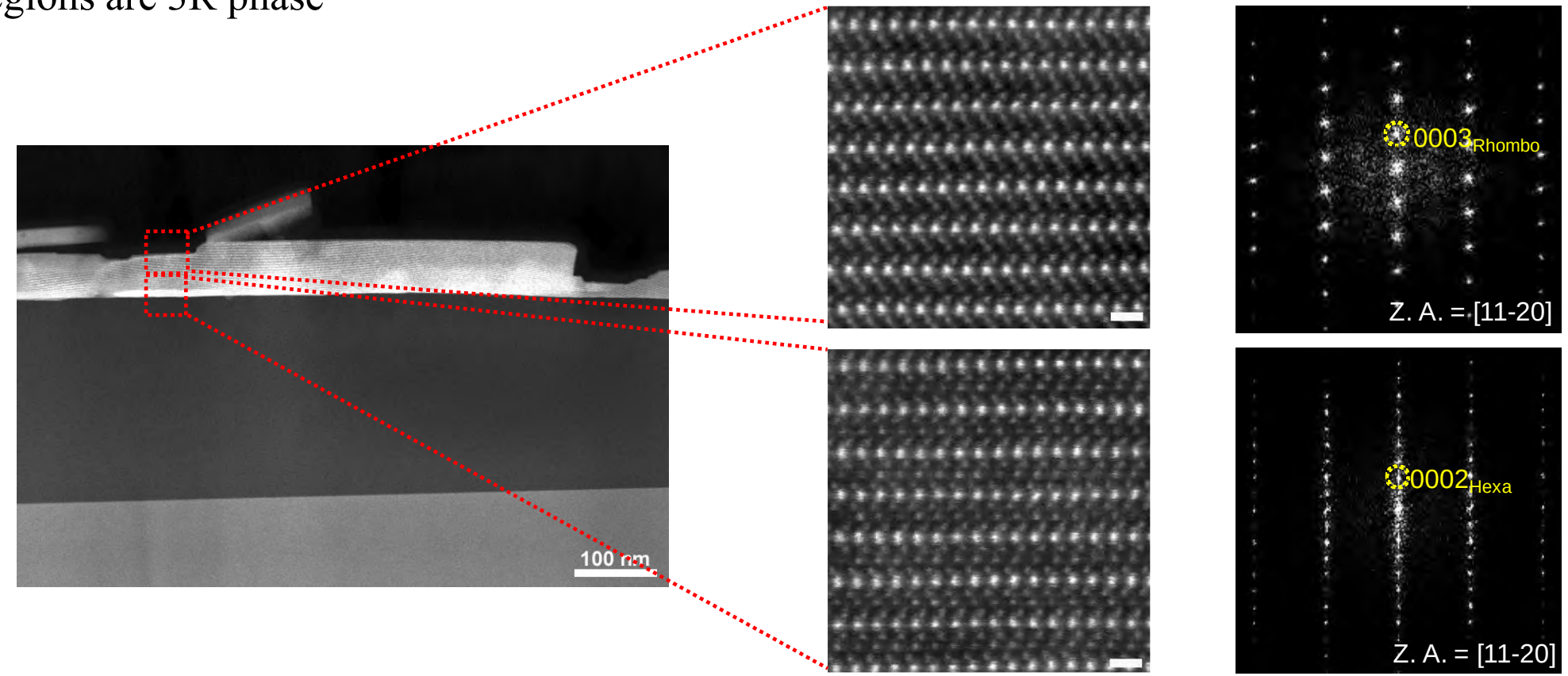






Cross – Sectional TEM of $Nb_{1.35}S_2$

Two different phases of NbS2 observed – thin regions ae 2H phase (metallic) and thick regions are 3R phase



$Nb_{1.35}S_2$

NATURE February 6, 1960 VOL. 185

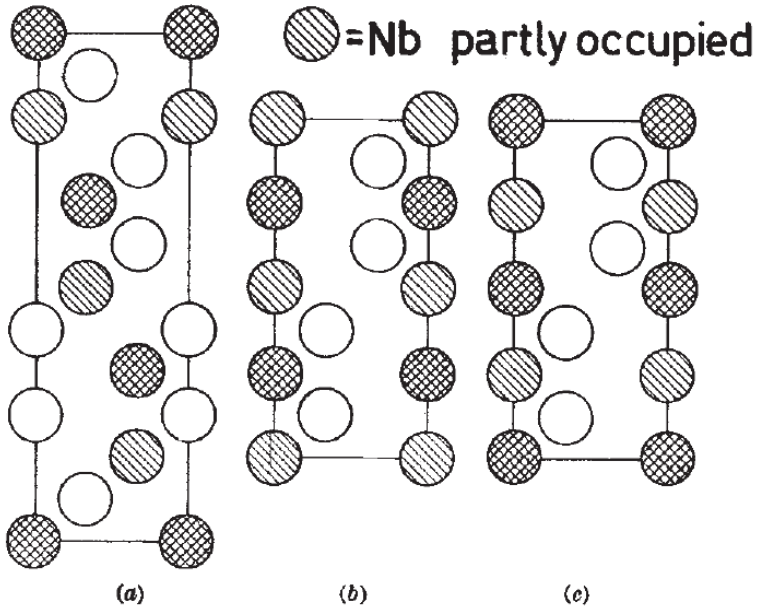
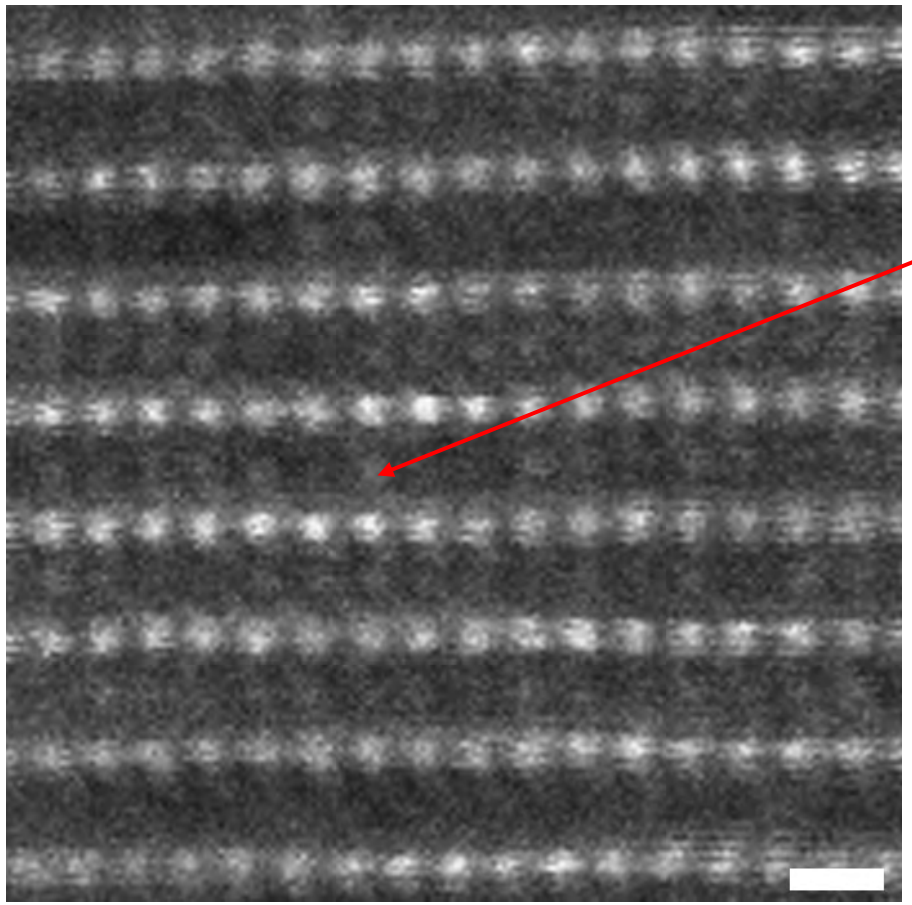


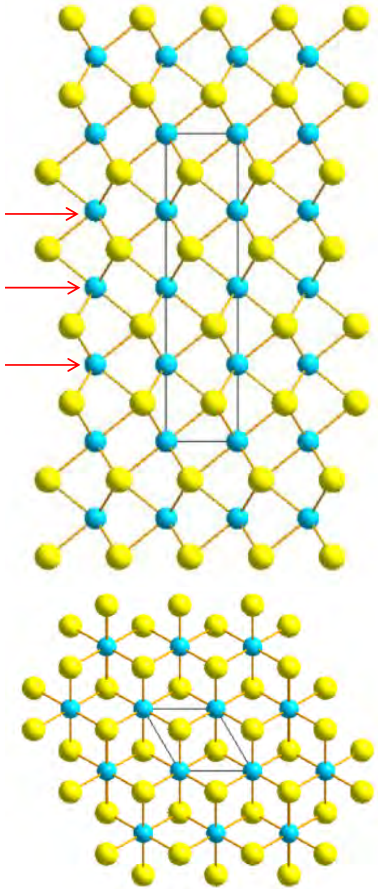
Fig. 2. Sections through the (1120) planes of (*a*) rhombohedral $Nb_{1+x}S_2$, (*b*) hexagonal $Nb_{1+x}S_2$, (*c*) one of the possible arrangements of $Nb_{2-y}S_2$

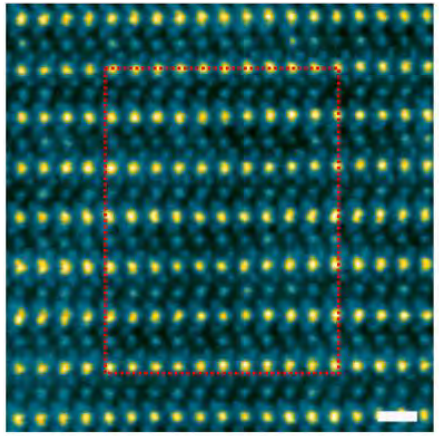
2H $Nb_{1.35}S_2$

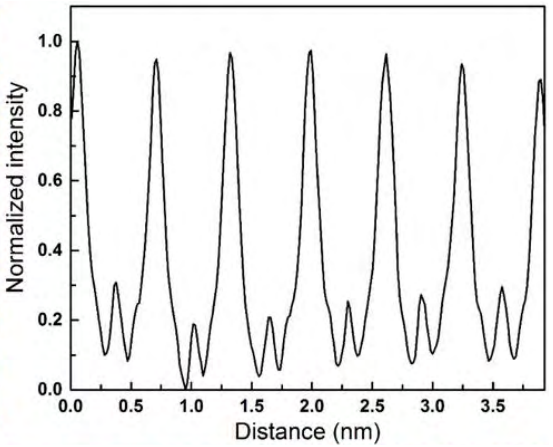


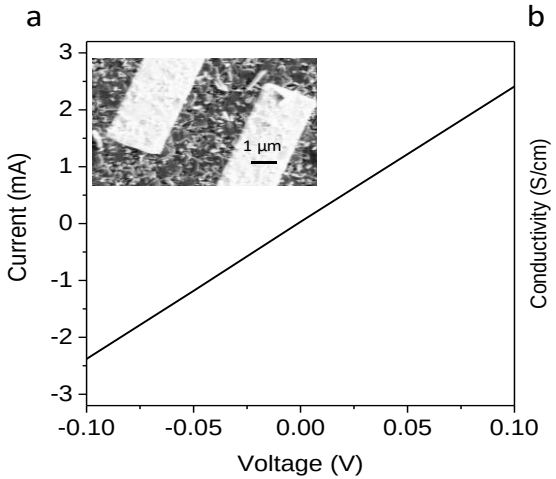
We can observe additional Nb layers in the hexagonal structure.

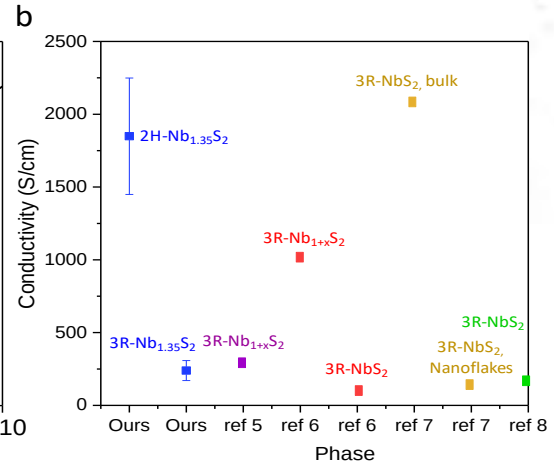
$Nb_{1.35}S_2$ for HER

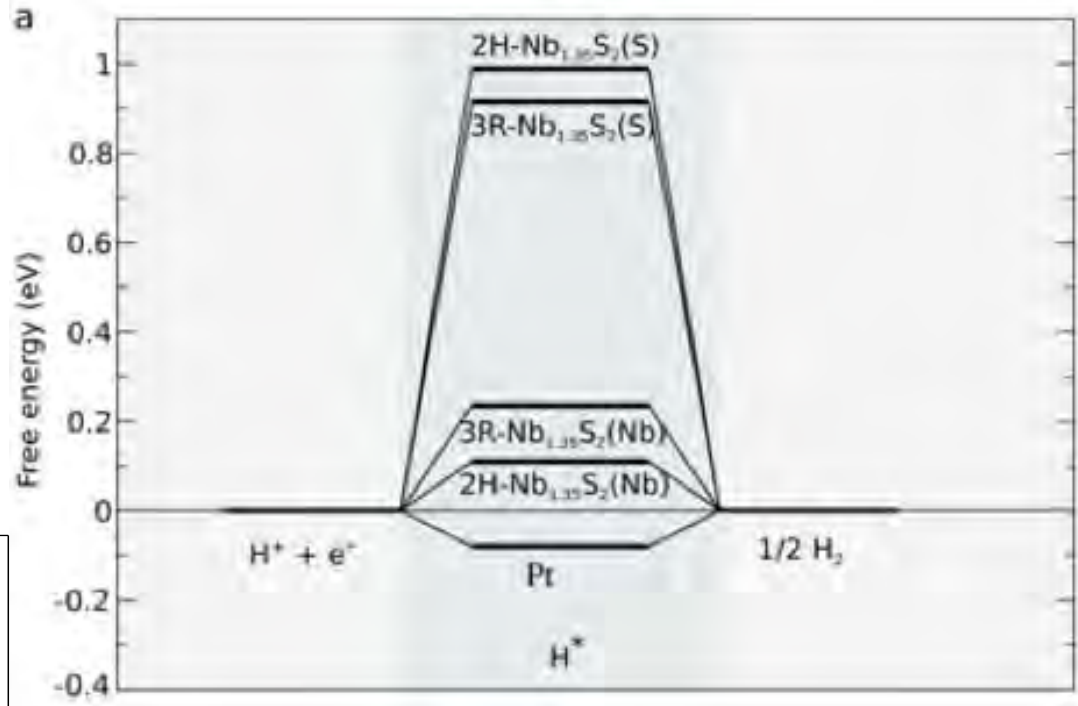




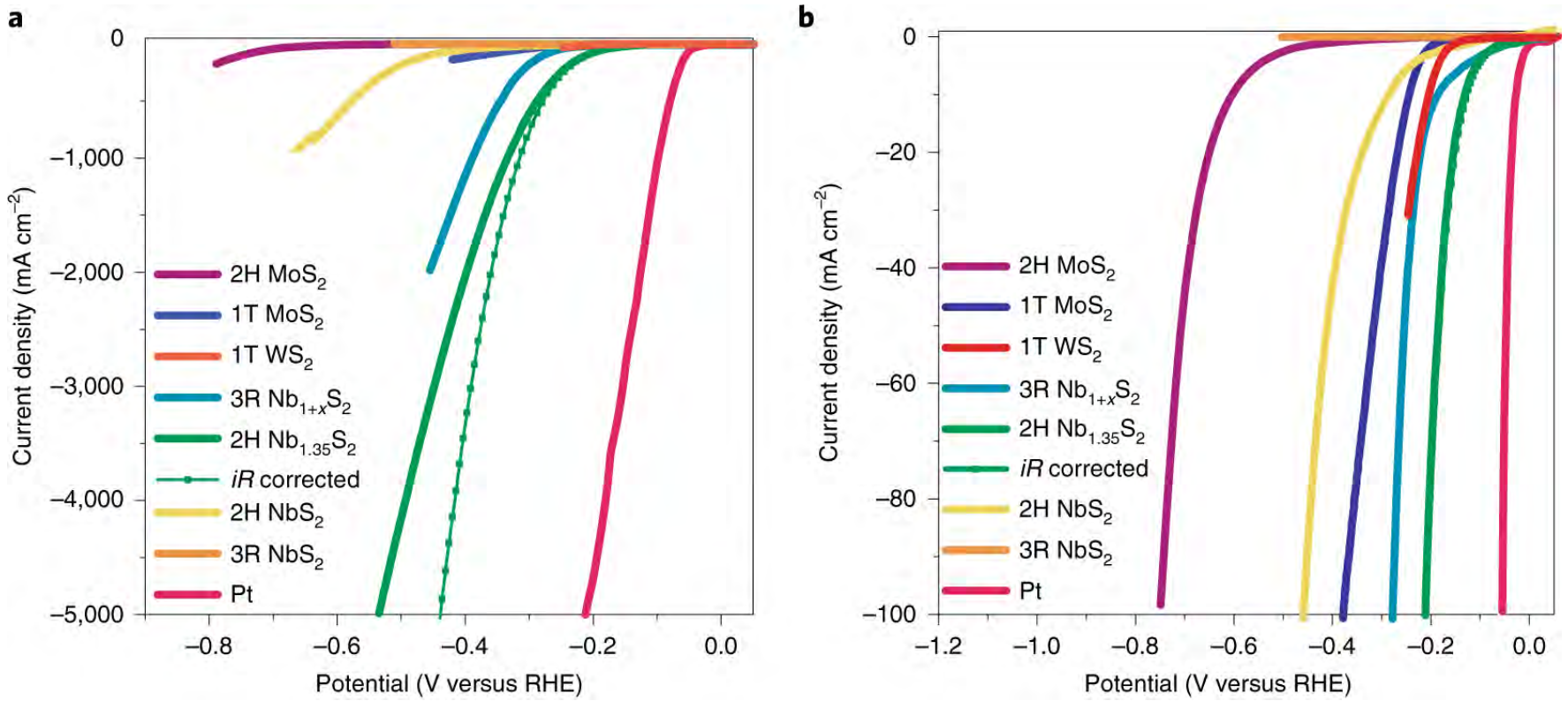






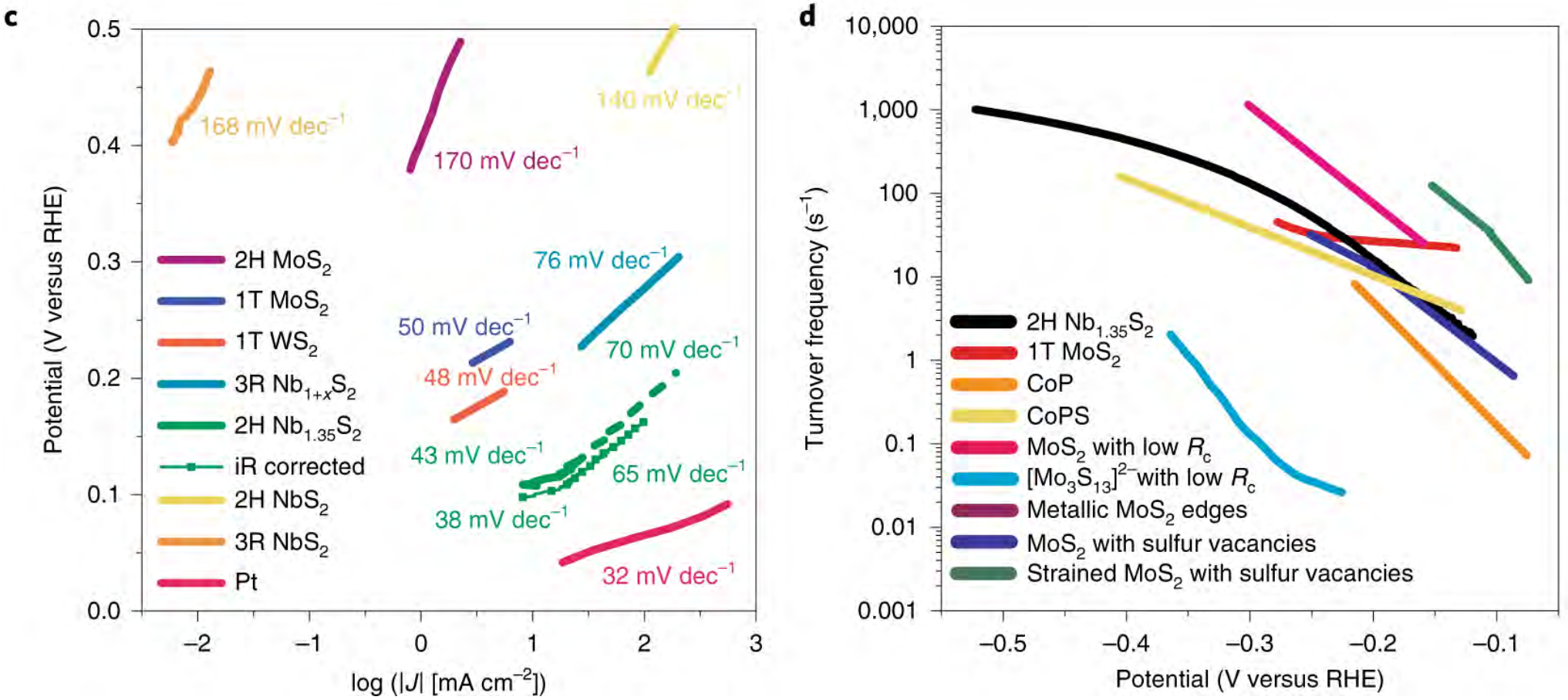


HER Properties of $Nb_{1.35}S_2$



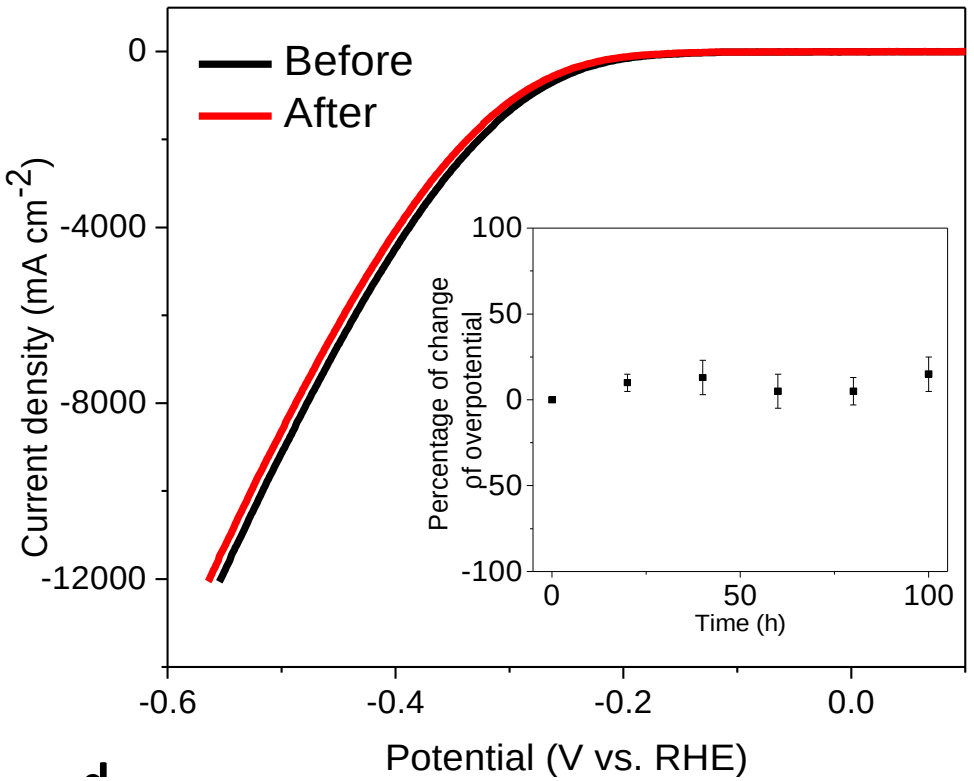
The rate of H_2 evolution reaches ~30 L cm^{-2} h^{-1} equivalent to 6 mmol h^{-1} cm^{-2} at 400 mV.

HER Properties of $Nb_{1.35}S_2$

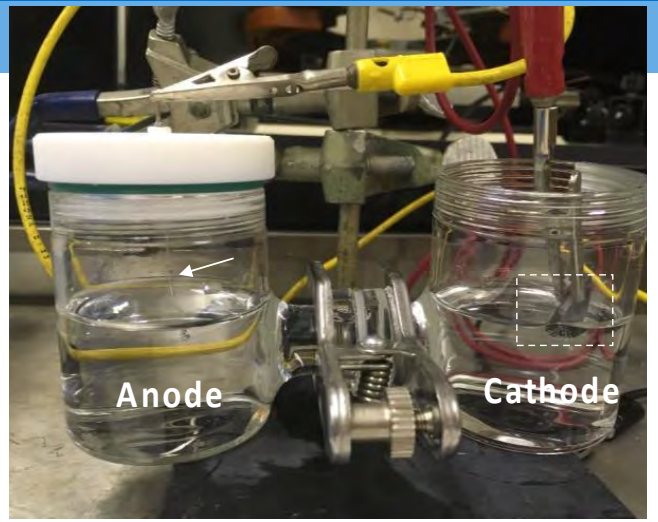


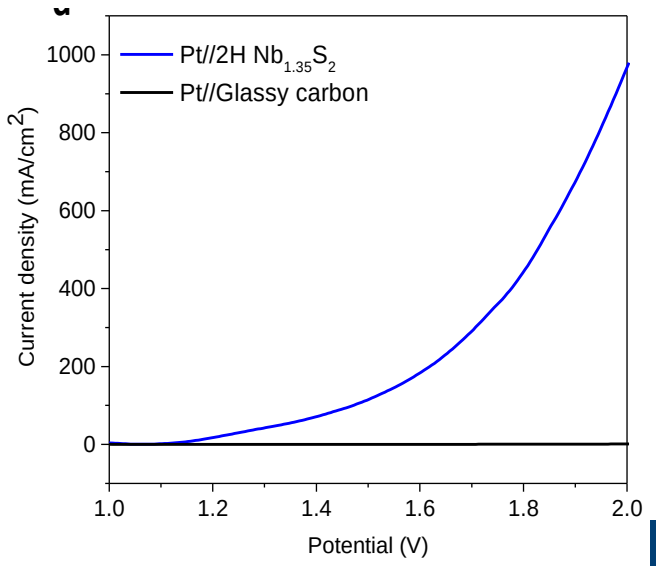
2H NbS_2 catalysts for large scale hydrogen production

❖ 2H Metallic NbS_2 catalysts



❖ 2H Metallic NbS_2 catalysts





❖ Real Electrolyzer with current density of 1A/cm^2 Demonstrated

UNIVERSITY OF CAMBRIDGE

Acknowledgements

Jieun Yang

Abdul Rahman Mohmad
UKM - Malaysia

Elton Santos
Univ of Edinburgh

Hu Young Jeong
UNIST

Thank You!

Companhia Brasileira de Metalurgia e Mineração (CMMB)

Charles Hatchett Award 2020 Panel

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*]

UNIVERSITY OF CAMBRIDGE