Is 3D/2D passivation a secret to success for polycrystalline thin-film solar cells?

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Overview

1 ‘High-performing’ thin-film photovoltaics

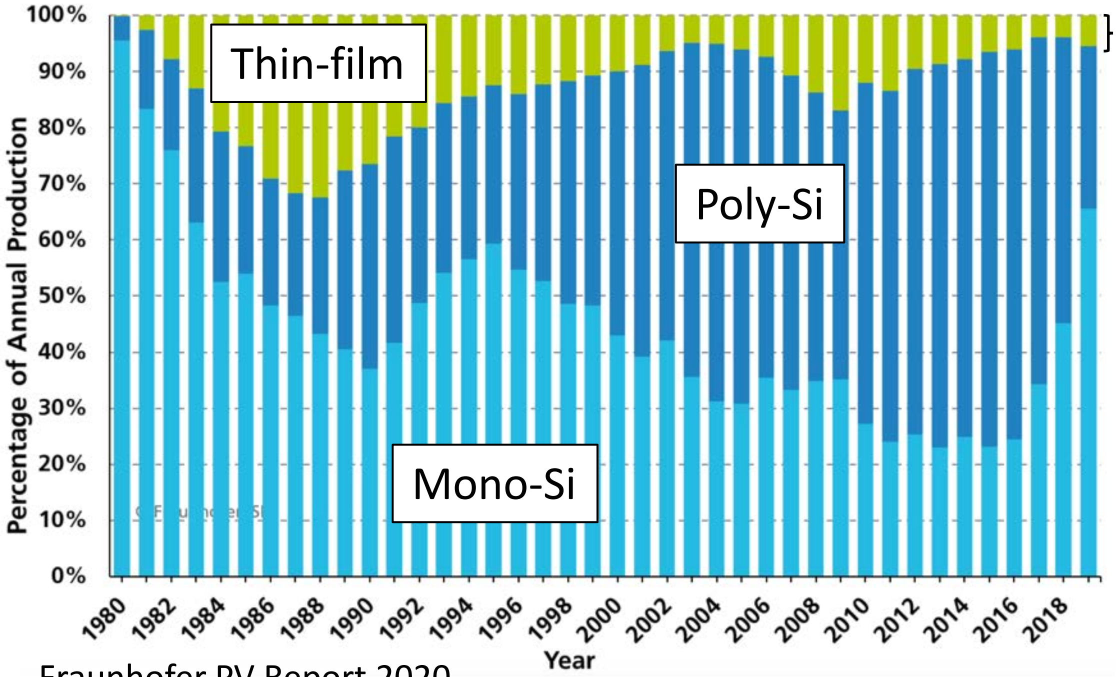
2 Advantage of 2D surface layers

3 2D layers in CIGS, CdTe, and perovskites

4 Improved lifetime and voltage in 3D/2D systems

5 Design rules for incorporating 2D materials

Thin-film photovoltaics



Fraunhofer PV Report 2020

cadmium telluride → CdTe; $CuIn_{1-x}Ga_xSe_2$ → CIGS; perovskite solar cells → PSCs

	Polycrystalline		
	CdTe	**CIGS**	**PSCs**
Annual production	> 5 GW/yr	> 1 GW/yr	~ 0 GW/yr
Record cell efficiency	22.1%	23.4%	25.5%
Growth order	superstrate	substrate	superstrate or substrate
Composition	II-VI	I-III-VI_2	Organic / I-IV-VII_3
Majority carrier concentration (cm^{-3})	p ~ 10^{14} (Cu) p ~ 10^{16} (As)	p ~ 10^{16}	n, p ~ 10^{14} - 10^{16}
Minority carrier lifetime (ns)	1 – 40	20 – 400	150 – 2,000

McGott et al. DOI: 10.1016/j.joule.2021.03.015

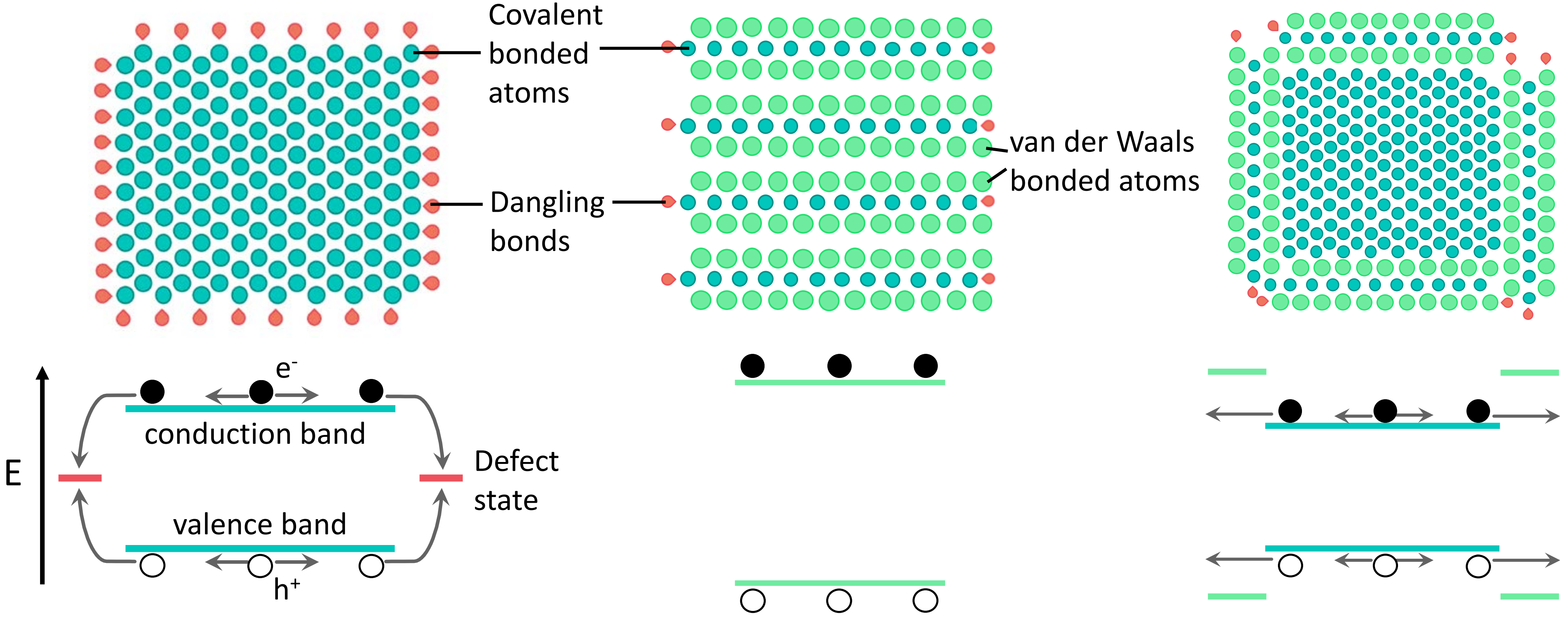
<u>Key Similarities</u>

- Inexpensive
- Rapid deposition
- **Polycrystalline**

Advantage of 2D surface layers

McGott et al. DOI: 10.1016/j.joule.2021.03.015

3D **2D** **3D/2D**



3D

- Defective surface → recombination
- Good charge transport in bulk

2D

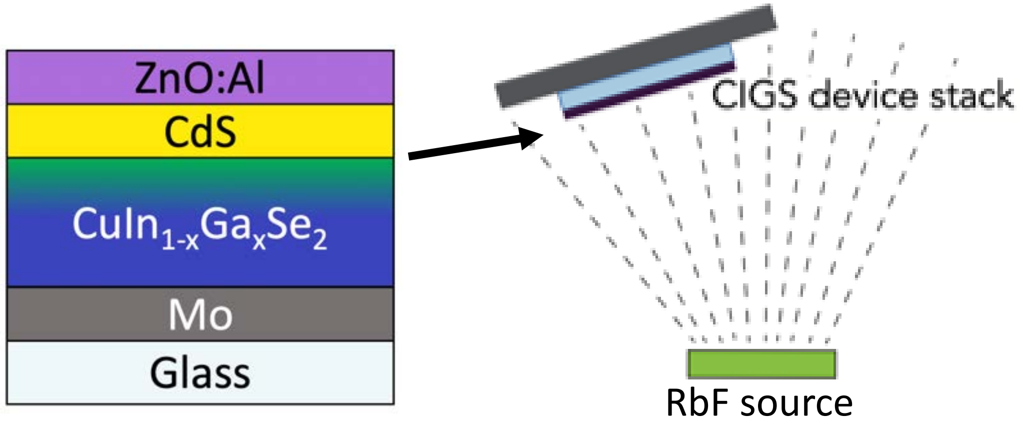
- Chemically passive surface
- Poor interlayer charge transport

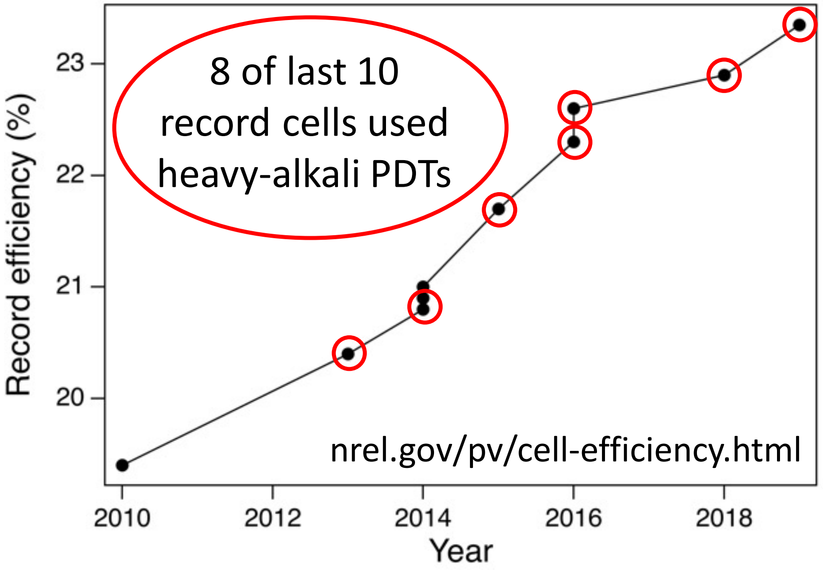
3D/2D

- Good bulk transport
- Passivated surface

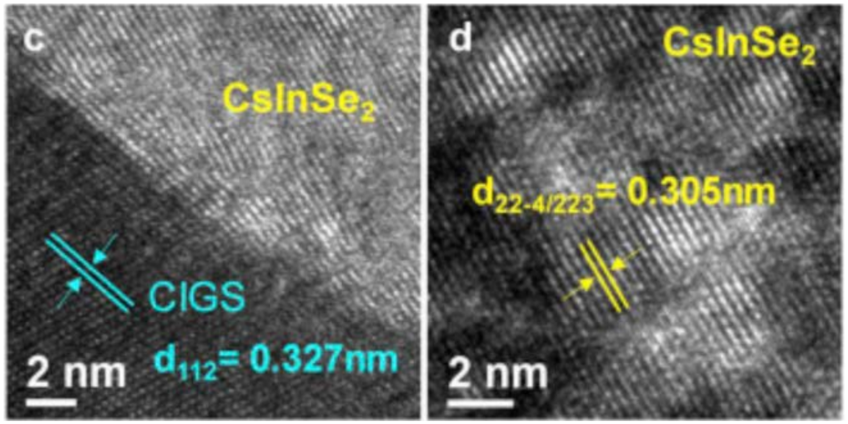
→ *Natural synergy*

2D $XInSe_2$ (X = K, Rb, Cs) in CIGS

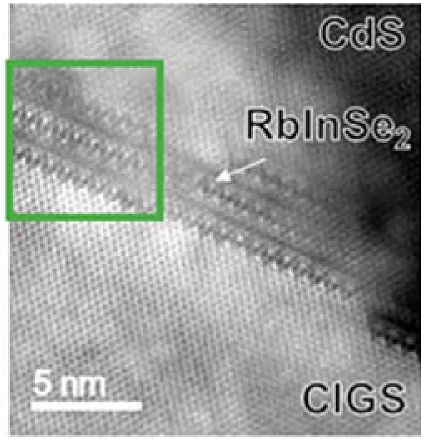




- Na-based post deposition treatment (PDTs) replaced with heavy-alkali (K, Rb, Cs) PDTs
- Alkali accumulation at absorber surfaces
- Direct evidence (TEM) for 2D layer formation

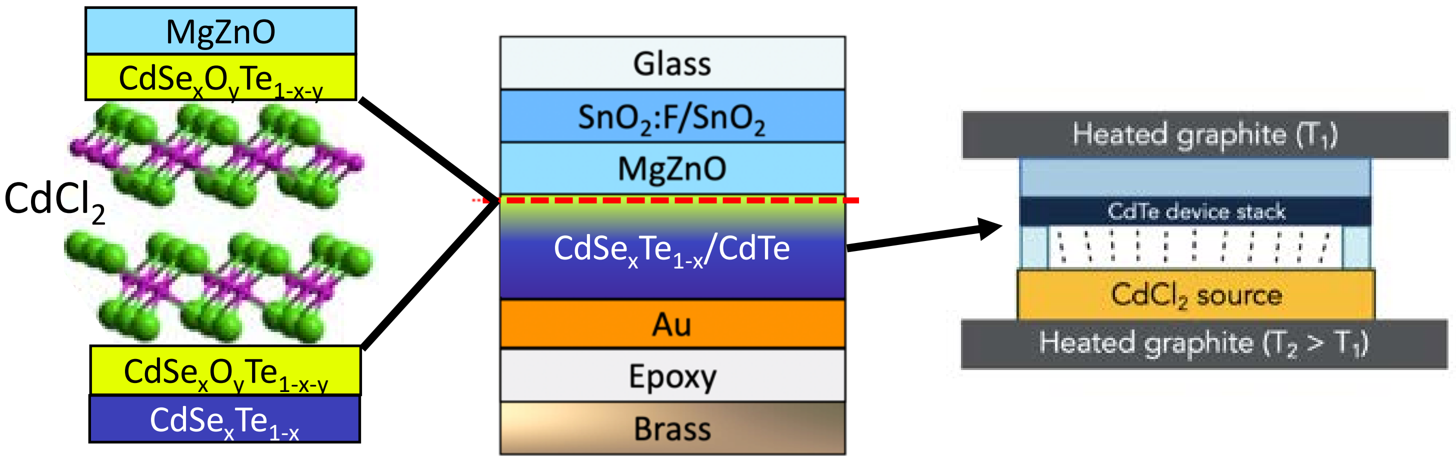


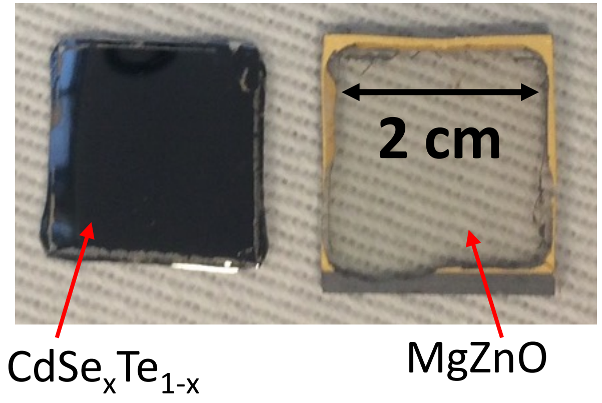
Lin et al. DOI: 10.1016/j.nanoen.2019.104299



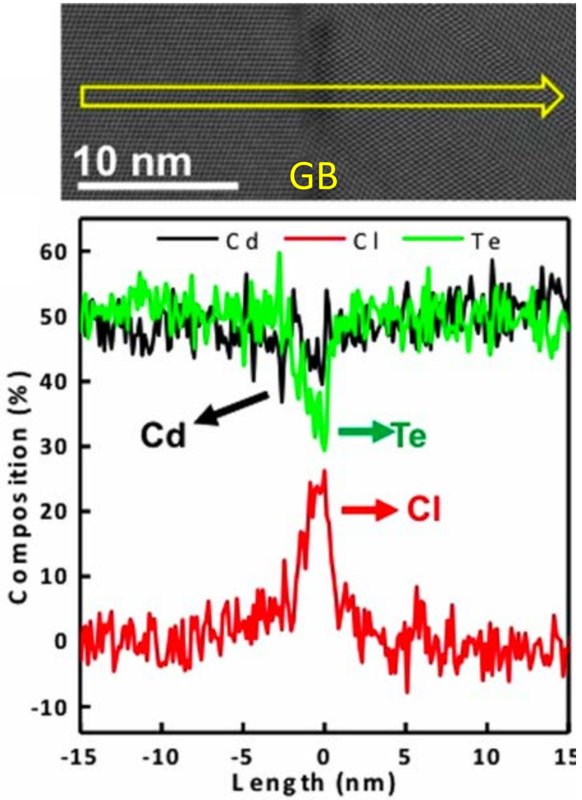
Taguchi et al. DOI: 10.1063/1.5044244

2D $CdCl_2$ in CdTe





- $CdCl_2$ anneal used in nearly every CdTe device
- Chlorine accumulates at grain boundaries and interfaces

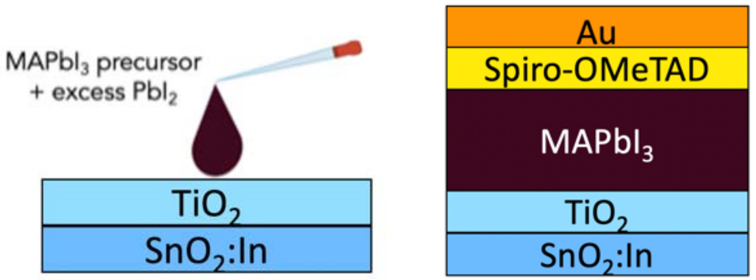


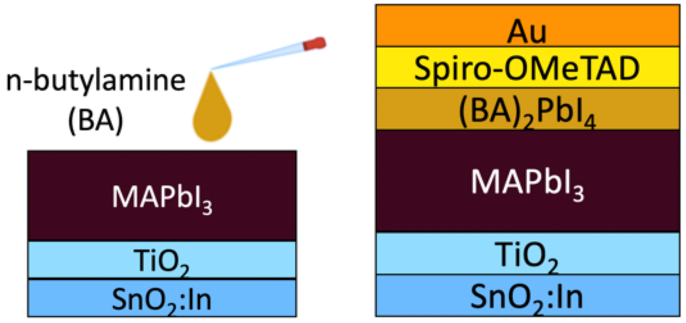
Li et al. DOI: 10.1103/PhysRevLett.112.156103

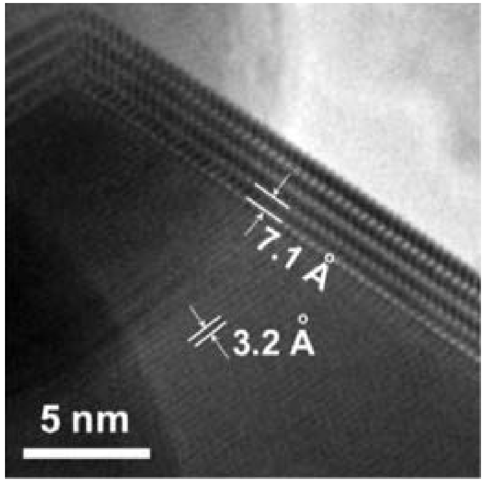
Cleave + surface analysis reveals chlorine in form of 2D $CdCl_2$

See McGott et al. DOI: 10.1016/j.joule.2021.03.015 for more details

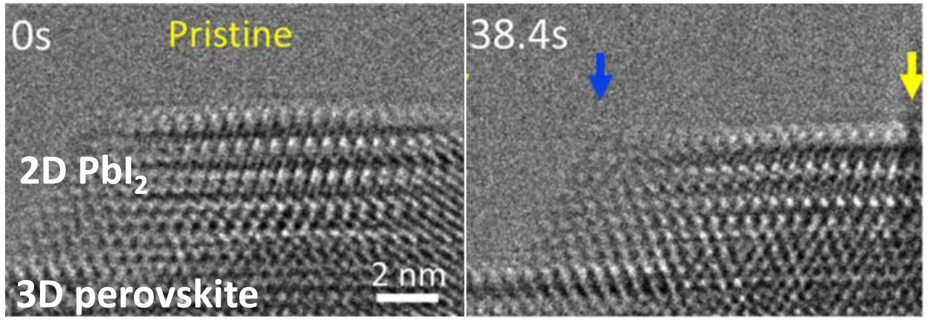
2D PbI_2 (& others) in PSCs





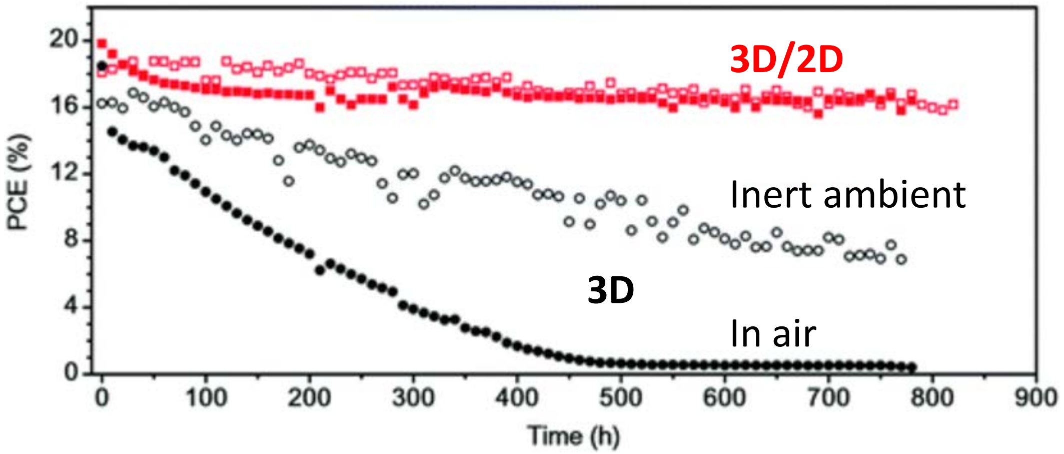


Tong et al. DOI: 10.1126/science.aav7911



Jung et al. DOI: 10.1021/acs.nanolett.9b02069

- Highest performing devices typically have excess PbI_2 in precursor
- Forms 2D PbI_2 capping layers
- PbI_2 accelerates degradation

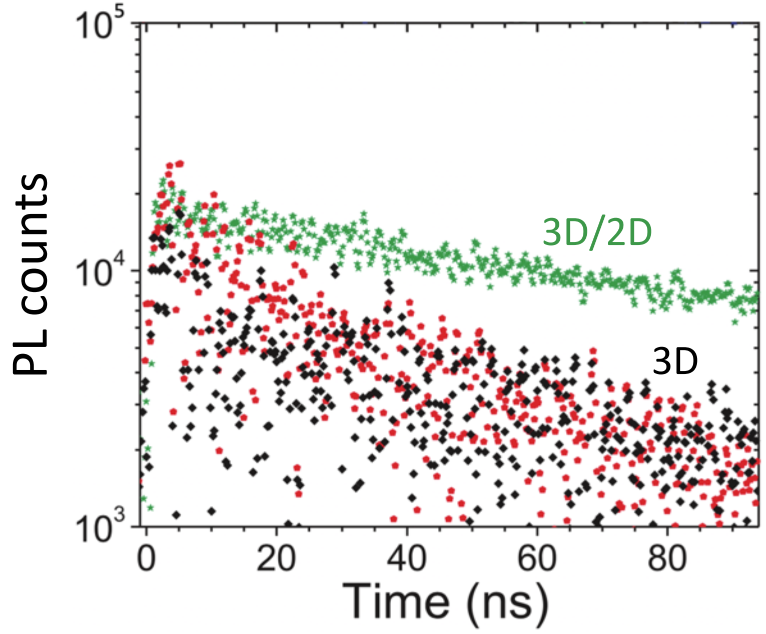


Taek Cho et al. DOI: 10.1039/C7EE03513F

Effect on carrier lifetime

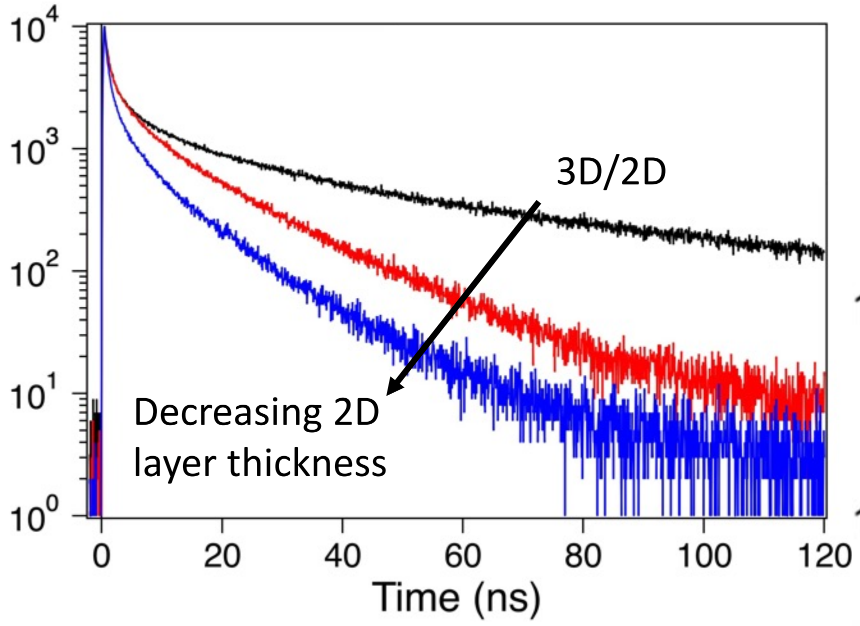
See McGott et al. DOI: 10.1016/j.joule.2021.03.015 for more details

CIGS



Muzzillo et al. DOI: 10.1016/j.solmat.2018.05.013

CdTe



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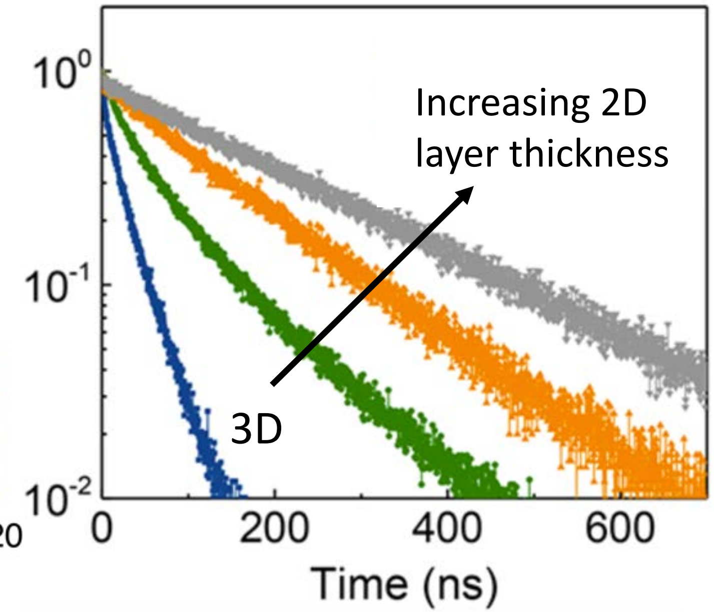
PSCs



Lin et al. DOI: 10.1021/acs.jpclett.7b02679

- 2D layer removed or added to single interface to limit bulk effects
- Time-resolved photoluminescence (TRPL) shows improved carrier lifetime with 2D layers for all three technologies

Effect on device performance

See McGott et al. DOI: 10.1016/j.joule.2021.03.015 for more details

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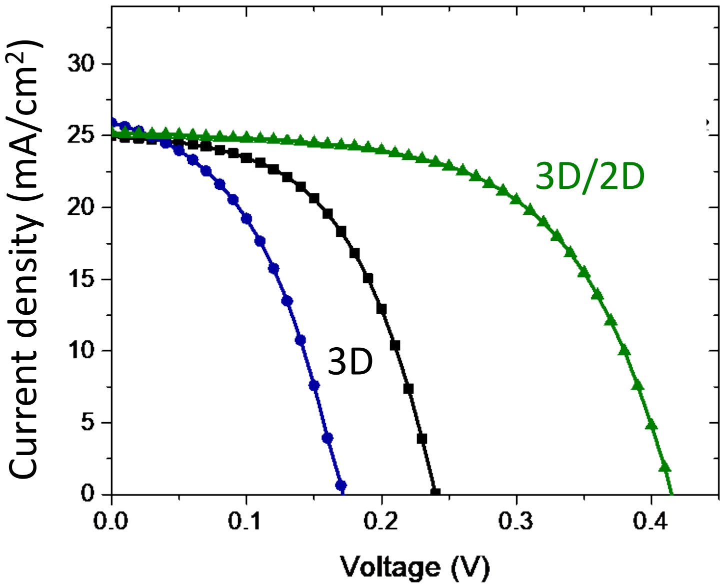
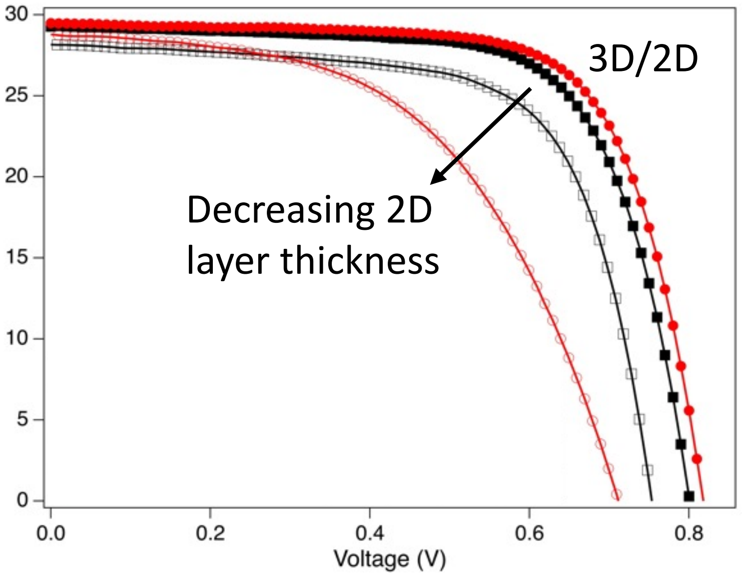


Muzzillo et al. DOI: 10.1016/j.solmat.2017.12.038

CdTe



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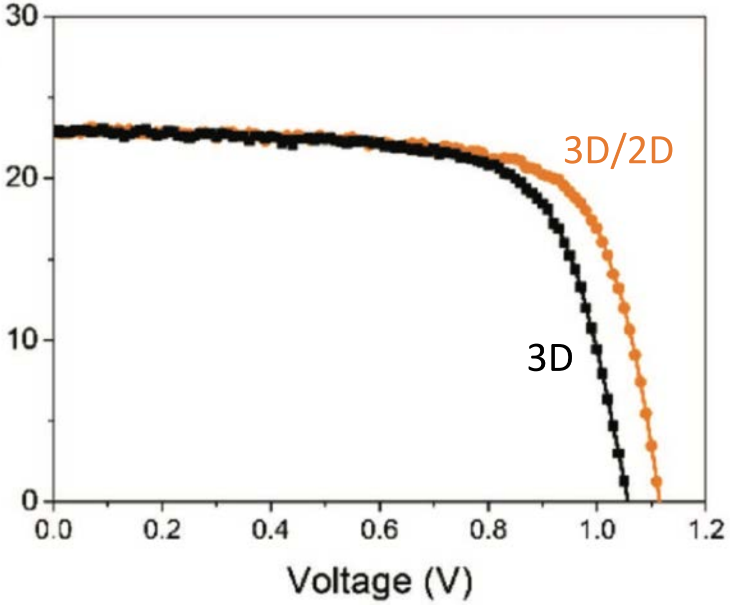

Chen et al. DOI: 10.1002/adfm.201706923

- Longer lifetime = less recombination = higher voltage
  - Seen in all three technologies with 2D layers
- 2D layer removed or added to single interface to limit bulk effects

3D/2D design rules

See McGott et al. DOI: 10.1016/j.joule.2021.03.015 for more details

Successful passivating agents should:

1) Terminate dangling bonds at surface
   - Transition from 3D→2D must also be passivated
   - 1D and 0D materials (e.g., nanotubes, C60) also satisfy
2) Target dominant defect(s) (i.e., anion or cation)
   - Ex: CIGS surface Cu-poor, should target Se (group III) dangling bonds
3) Not introduce mid-gap states
   - Preferable if 2D bandgap > 3D bandgap
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   - Precursor dissociation energy should be low
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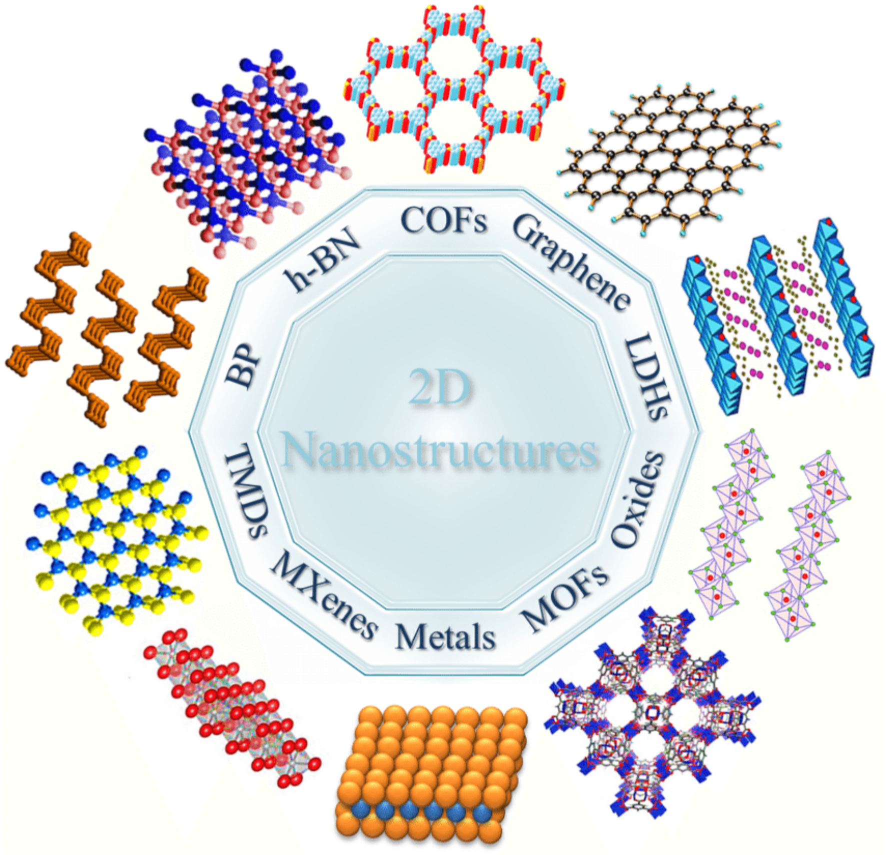

Azadmanjiri et al. DOI: 10.1039/C6RA20050H

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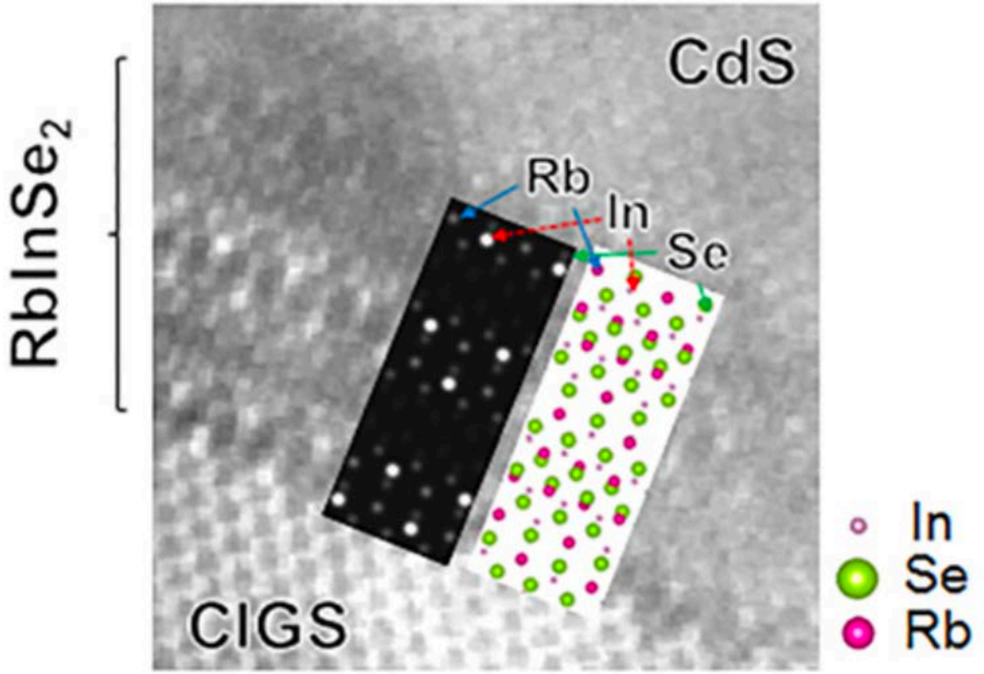

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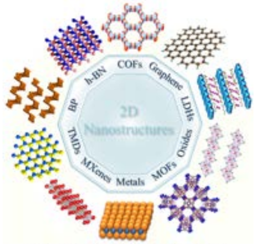

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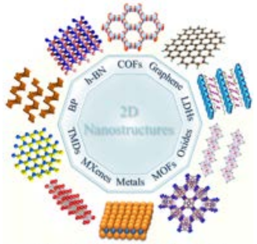

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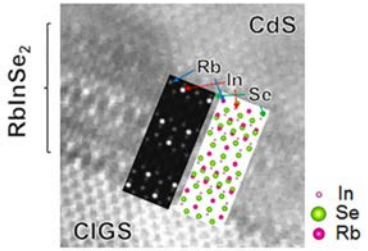

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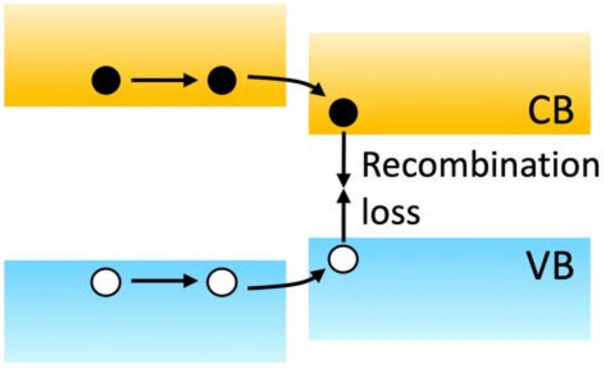
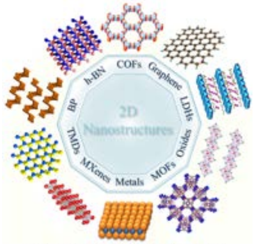


	E_{gap} (3D bulk)	E_{gap} (2D layer)
CIGS	1.0 – 1.7 eV	2.0 – 3.22 eV
CdTe	~1.5 eV	5.8 eV
PSCs	~ 1.6 eV	≥ 2.3 eV



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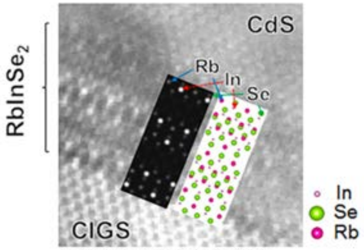

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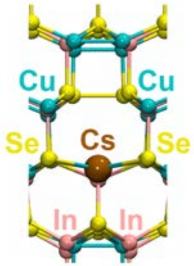

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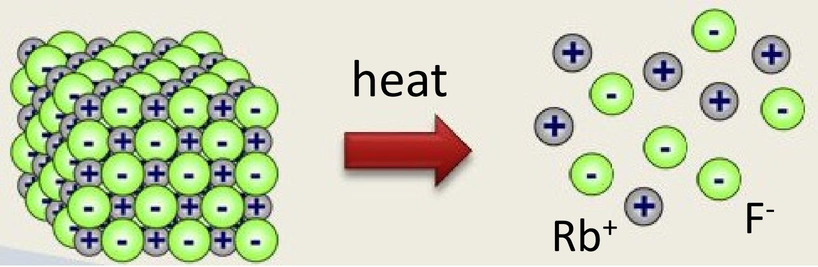

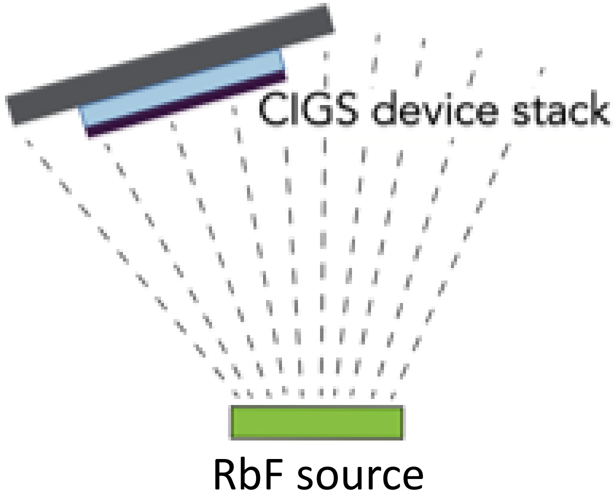

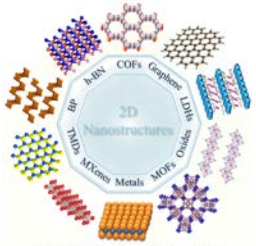

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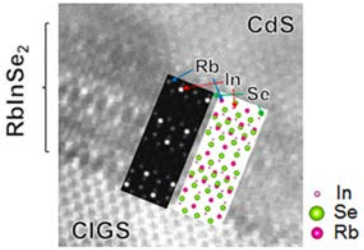

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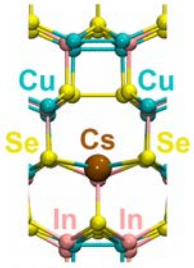

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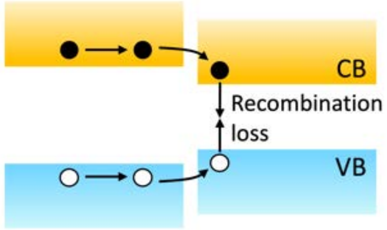

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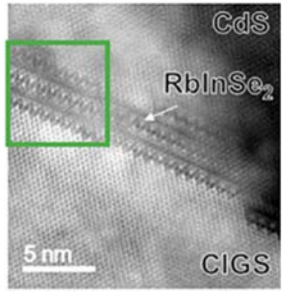
More details: 10.1016/j.joule.2021.03.015

CIGS



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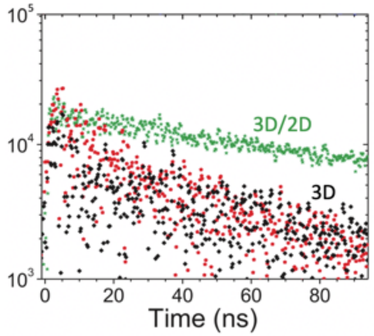

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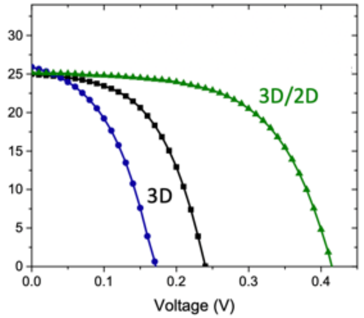

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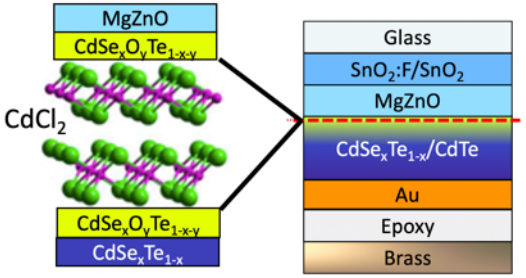
CdTe



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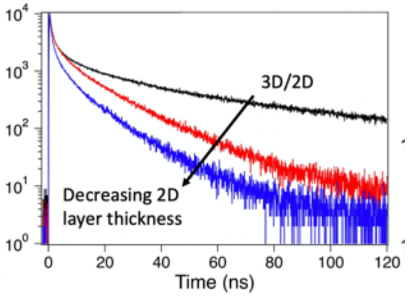

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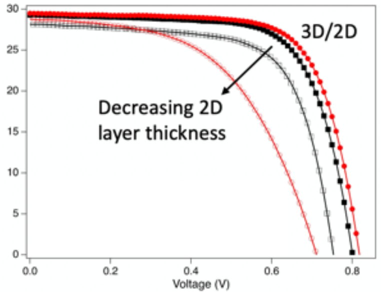

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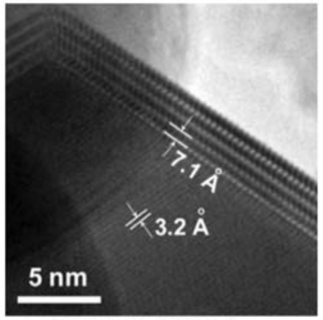

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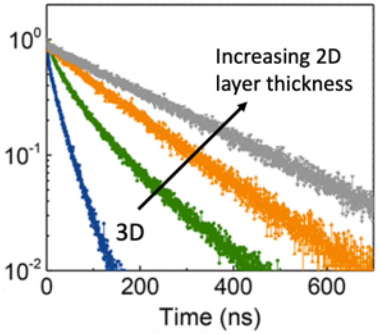

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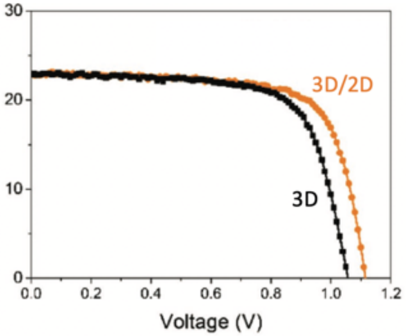

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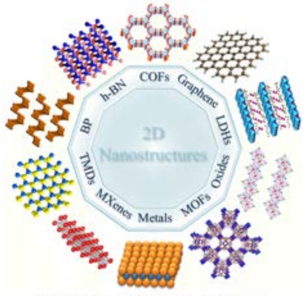
3D/2D design rules



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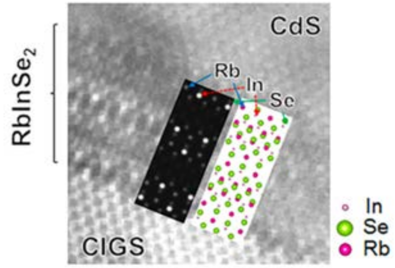

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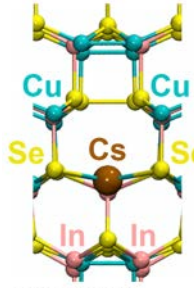

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