

Long-lived Perovskite Solar Cells: Fixing the Problems

From Bulk, to Grain Boundary, to Interface

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- **What is PV, & why perovskite PV?**
- **Recent progress of PVSF at UCLA**
- **Prospects of PVSF**

The DOOR, it opens the future!



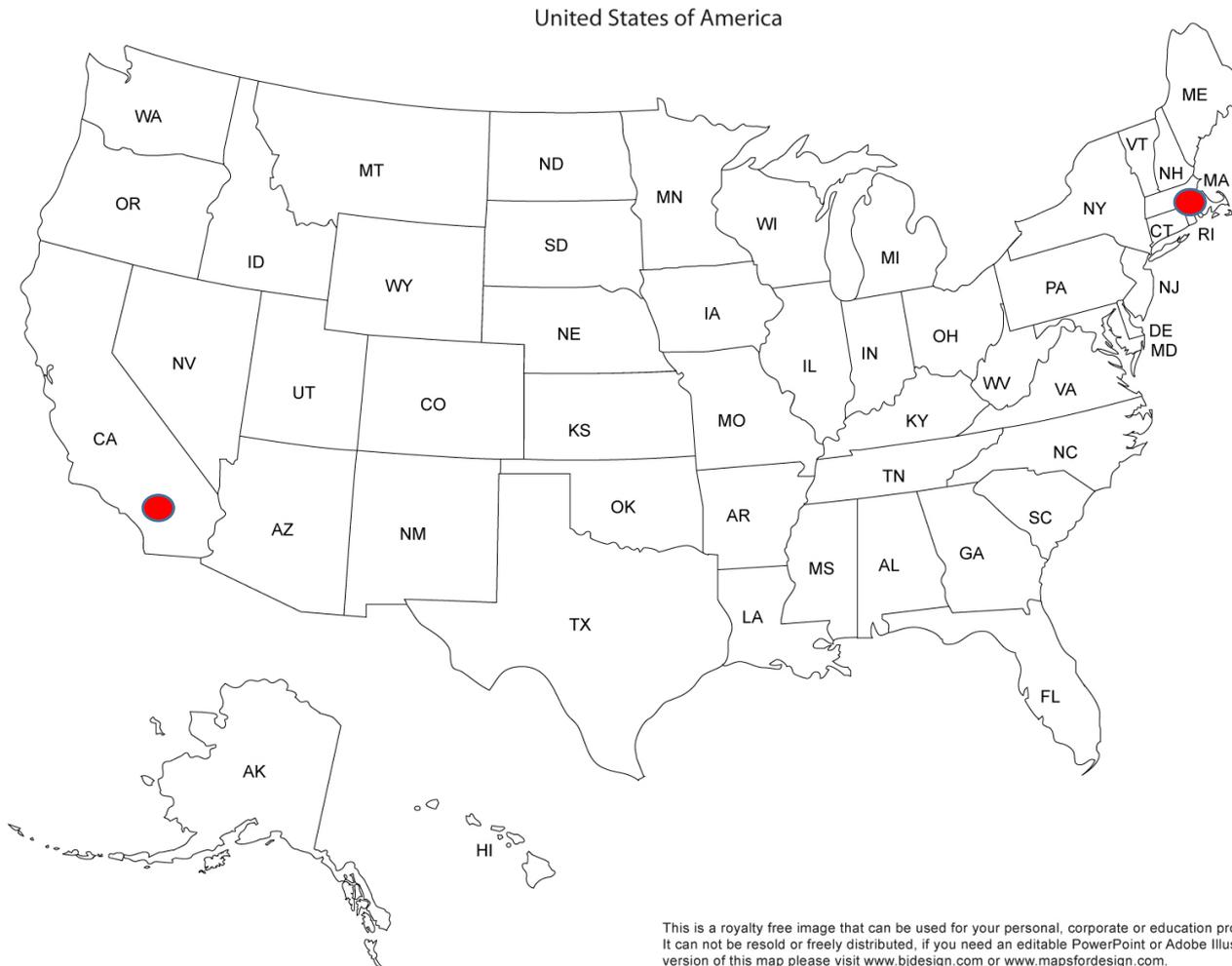
走

人走活

Risk taking, really?

Be Dynamic &
Think out of the box.
Be yourself

楊陽的求學與工作經歷



1985 – 1991 Massachusetts
MS degree and PhD degree

1991 – now: California

1991-1992: Postdoc, UC-Riverside

1992 – 1996: Staff Scientist
UNIX Corp.

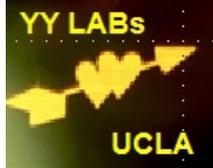
1997 – now : UCLA, Professor

2019 – 2020 中國杭州,

Dean of Engineering School
Westlake University

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分享3+1個故事



- 哪裏跌倒，哪裏爬起來：我大學重考經驗 (1977-78);
- 如何把劣勢變成優勢？我在美國職場的準備 (1986-96);
- 占領戰略製高點：UCLA 的有機光伏的藍海策略 (以及我如何帶學生，建立我課題組的文化。) (2008-2018)
- 二次創業：我的選擇不見得都是對的，但是，...how to reinvent myself is the key ...

*我們沒辦法預言未來，我們只能回顧過去，來分享我的故事。但是，當年在做這些決定的時候，心裏是害怕的不得了。

We can only connect the dots when we look backward. Steve Jobs, 2005

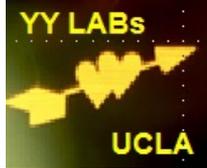
Story-1. 哪裏跌倒，哪裏爬起來：

我的大學重考經驗 (1977-78)

Facts to be shared: 1977 大學聯考英文高標準是71分。
可是我的英文成績只有17分。

怎麼辦？

Trust your own instinct - 我的高中英文故事



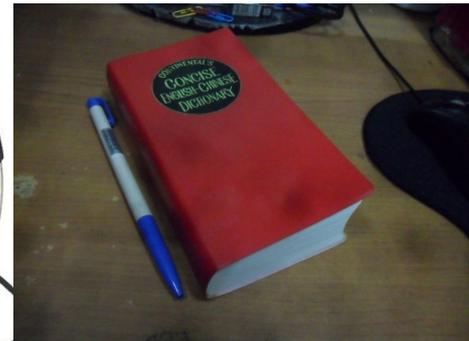
我工作很賣力, 就是**不得其門而入**, 英文補習也沒有用, 方法不對結果是自信心全部失去

I have to do something **dramatically different** to save my English. – Find my own way to deal with it.

1977 大學聯考英文: **17** 分; 高標準71分。

1978 大學聯考英文: **51** 分; 高標準35分。

- 自己設計教材 以及方法。
- 四個月的時間聚焦一件事情
- 注



4 months efforts, benefits my whole life

What did I learn?

- 我可以靠自己 **走** 出一條路；
- 不必相信別人的偏方，相信自己的能力！
- 這個經驗對我以後到美國求學就業，有深遠的影響

Self-confidence: 一次又一次被打倒再爬起來累積起來的。

Story-2: 把劣勢變成優勢



Facts to be shared: 1985 我來到 U-Mass Lowell. U-Mass Lowell 物理系當年排名是全美國200名。

怎麼辦？

Easy choice, hard life; Hard choice, easy life.

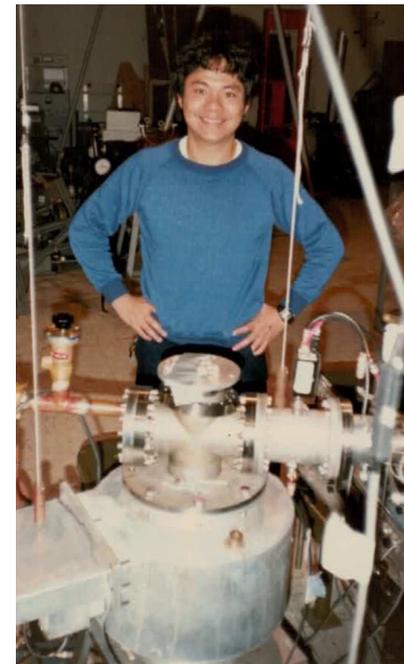
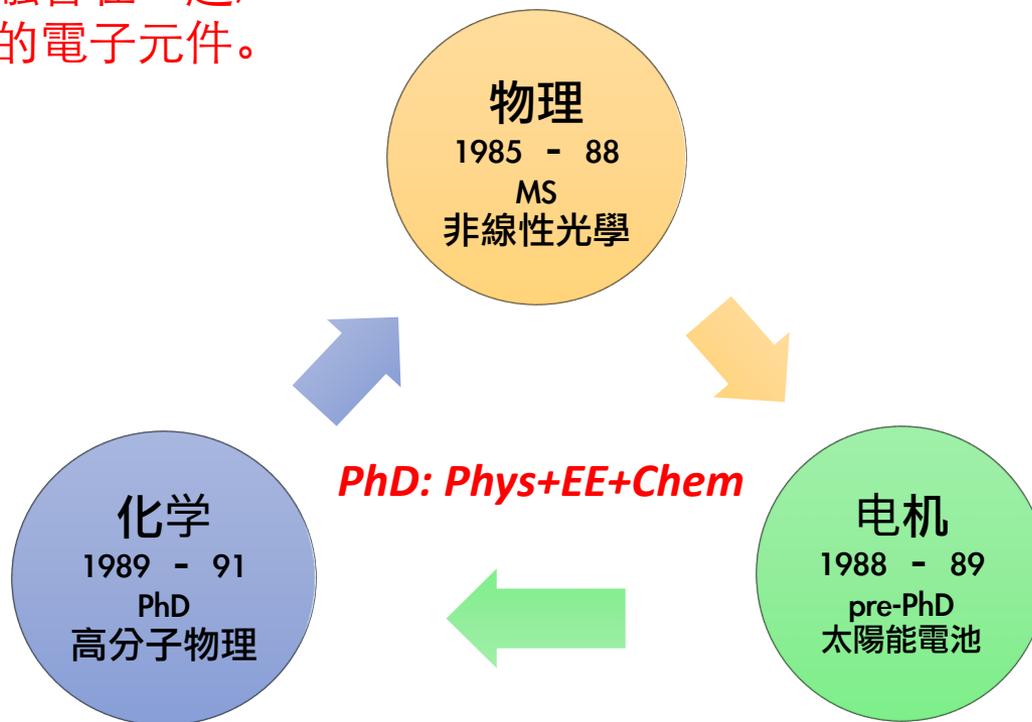
十年磨一劍：我在美國職場的準備工作(1986-1996);

博士學位經歷了三個課題組：



走

我發現我可以把半導體的和高分子融合在一起，來做高分子的電子元件。



我很喜歡半導體，但是這是個必須要做痛苦的決定。

因為我不想被卡脖子。

追逐夢想, 不輕易妥協

1991, 拿到博士學位之後, 我有好幾個工作機會

麻州: \$45K permanent job + 綠卡 + 公司股票

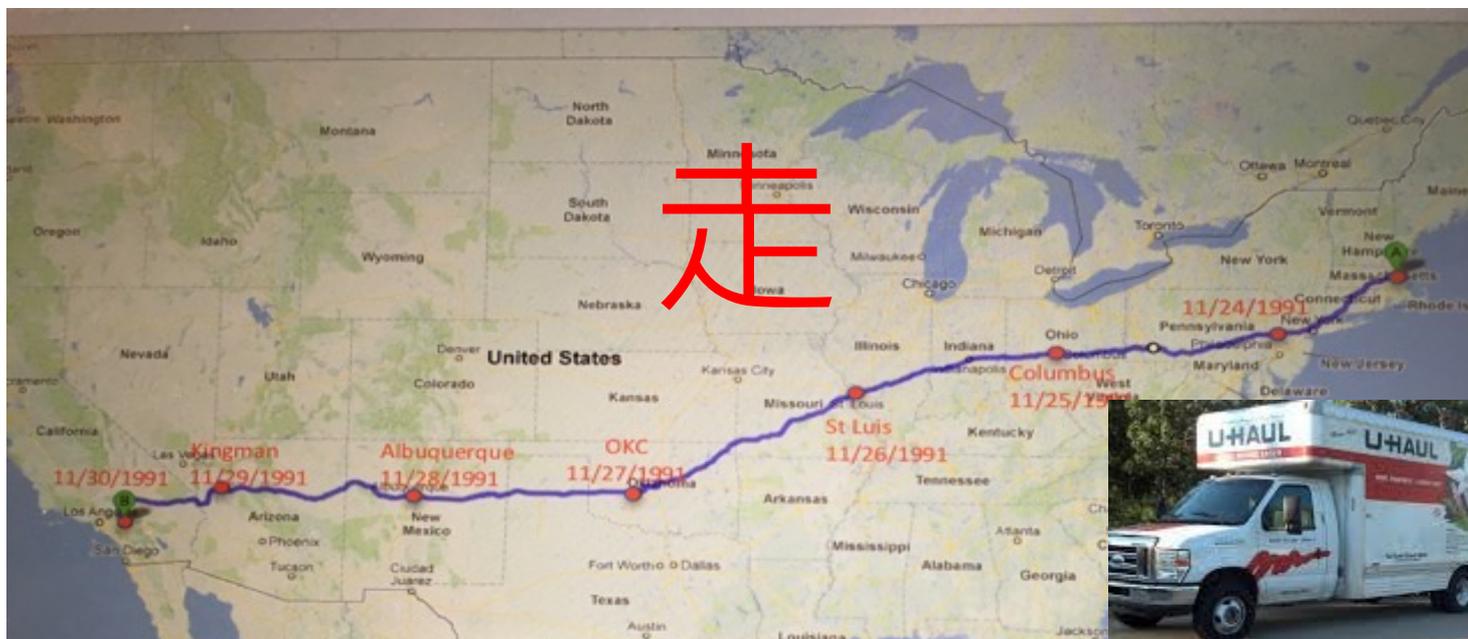
賭不賭?

VS



加州: \$22K postdoc, 沒有綠卡, 也沒有股票。

再加上還要自己開車5000公里



開車5000公里，沒有用倒車檔？



假如陷入困境, “走”, 是一個很好的選項

- 1991-92 Postdoc UC-Riverside (**only 10 months, why?**)
- 1992-96 tech-staff in UNIX Corp. (Santa Barbara).



做學問既要寬廣又要深，
From 1986-1991 (寬廣) & 1991-1996 (深度)

In 1997, join UCLA as Assistant Professor,

- 1998 Associate Professor, 2002 Professor, 2011 Tannas Jr. Chair Professor

1997年一月份正式加入UCLA



- Facts to be shared: **100,000美金的啟動經費**，還有**35平米的實驗室空間**
- **我絕對不做和我以前老東家類似的研究課題。**
- I need money, badly; and I need new ideas.



The world first successful inkjet printing OLED device. We received **\$1M of grants in 1998**

UCLA 的有機光伏的藍海策略

我們如何開始有機光伏的研究？

- 2001~02年, 交通大學陳方中教授剛完成博士論文, 我請他做計劃, 必須能讓人眼睛一亮, 但是也要符合我們的有機光電研究。我向他提出**有機太陽能電池計劃**;
- 後來我們拿到了**30,000美金的科研經費**。
- 我們後來用這筆經費請來了**李剛做博士後**。2005, 他做出了一個很重要的工作, **我們的文章被引用了超過6000次**。李剛是交通大學教授。
- 回顧過去, 我們**有機太陽能**, 成立了兩家公司到現在, 一共拿了超過了千萬美金的經費。

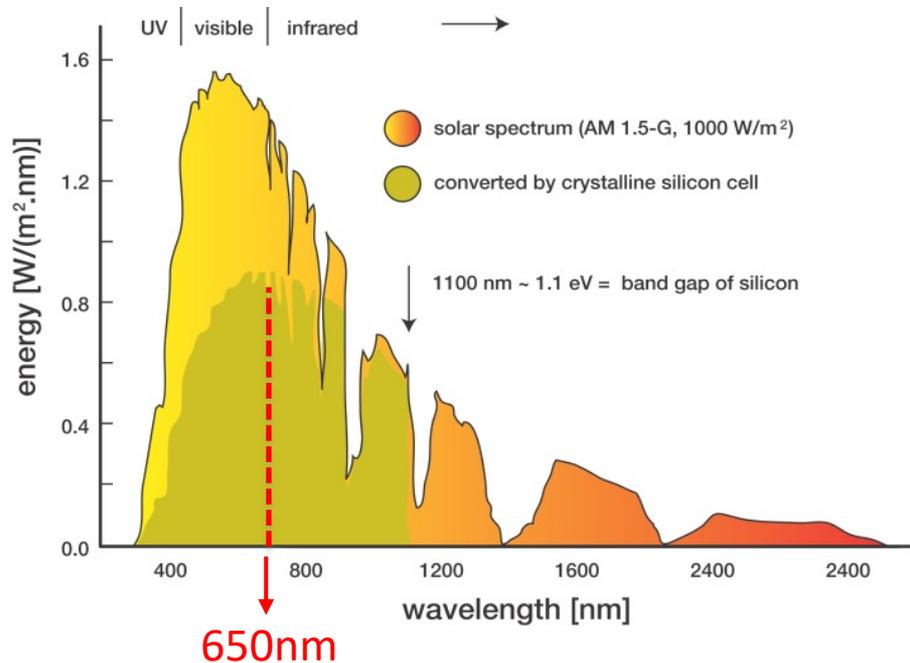


我們在2006/07年就已經站在OPV的世界頂峰的位置

Solar Spectrum

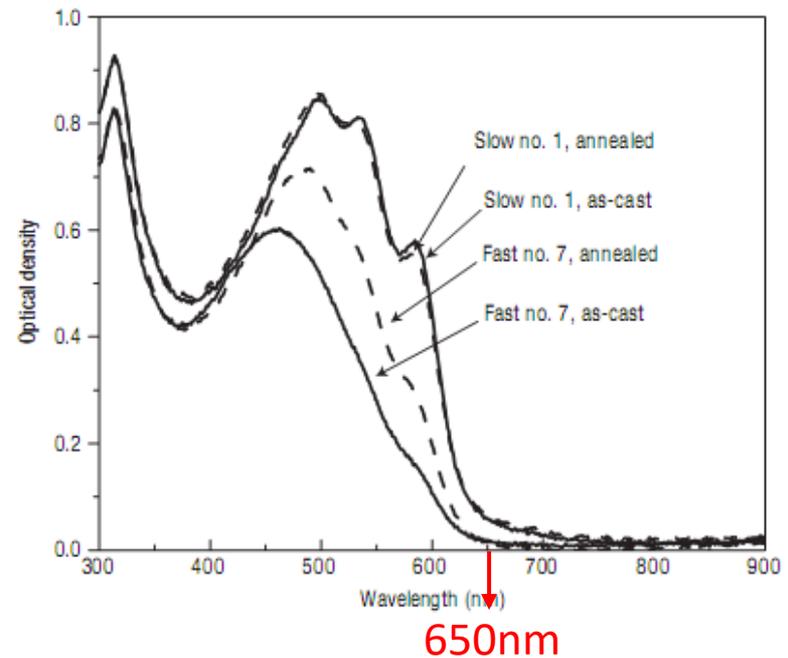
Standard used for measurements:

- Air Mass 1.5 (Sun at 42° of elevation)
- Irradiance ~ 1000 W/m²



P3HT:PCBM system

- Absorbs mainly in the visible spectrum
- Our lab has been researching novel **low-bandgap materials** to absorb more of the infrared spectrum

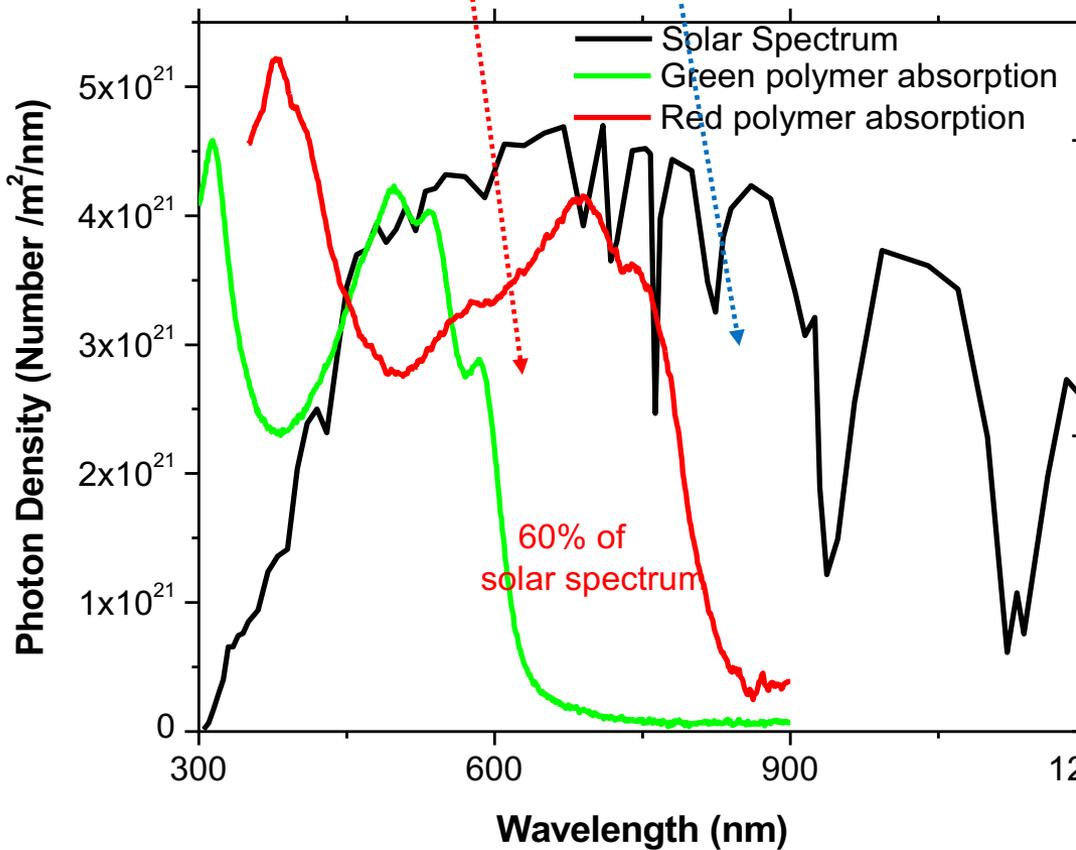


- 人無我有 → • 藍海
 - 人有我優 → • 紅藍海
 - 人優我**走** → • 紅海
- ↓
- “人無我有” 的藍海

走, be dynamic

YY Lab 在2007/08年的戰略思維

搶占“紅外線”戰略高地

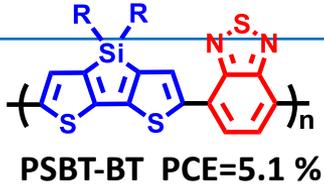


寶樂添的故事

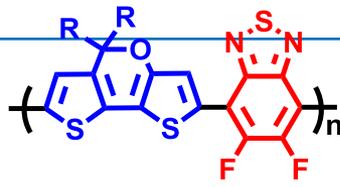


0.5 Ⓢ
從一開始我就和LT說我沒辦法指導他的化學，但是我可以指出大的方向。你願意來嗎？（賭上一把嗎）？

YY課題組合成的紅外線材料



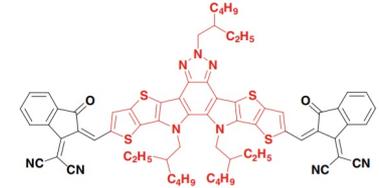
Prof. JH Hou



Prof. LT Dou

Nat. Commun. **2013**, 4, 1446.

Acceptor



Y1-Y3 Acceptor

Nat. Commun. **2019**, 10, 570.
Adv. Mater. **2019**, 31, 1904215.

First IR Polymer

IR Polymer Strategy

First Certified OPV efficiency over 10% (Tandem)

Ternary OPV device

(*Nat. Photon.* **2015**, 9, 190)

2012

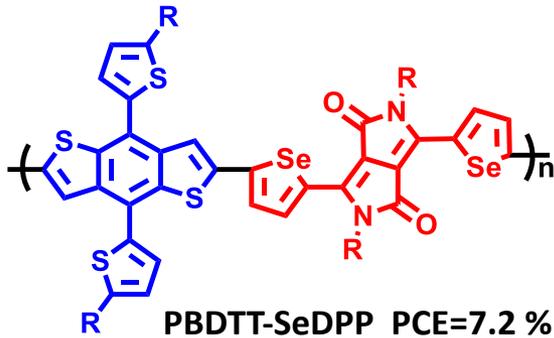
2015

2008

2013

2019

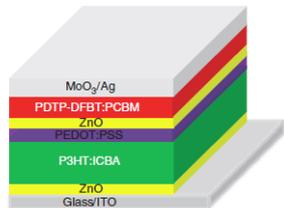
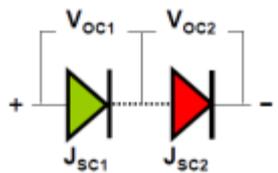
900-1000 nm IR Polymer



Adv. Mater. **2013**, 25, 825–831.

Achievements of UCLA Organic Photovoltaic project

150篇文章發表，超過50,000次的引用，平均一篇文章超過350次的引用



Highly Efficient Tandem Cells Transparent OPV

Nat. Commun., 4, 1446 (2013), cited 2566 times

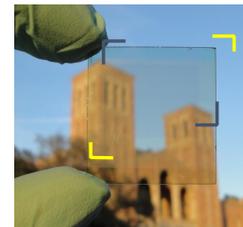
Nat. Photon., 6, 180(2012), cited 1395 times

Adv. Mater., 21, 1 (2009)

Adv. Mater., 21, 4238 (2009)

2013

2019
2018



ACS Nano, 6, 7185 (2012)

2012

2010

2009

Low Bandgap Polymers

Nat. Photon., 3, 649 (2009), cited 2993 times

J. Am. Chem. Soc., 131, 15586 (2009)

J. Am. Chem. Soc., 130, 16144 (2008), cited 1106 times

Vertical Phase Separation

Adv. Funct. Mater., 19, 1227 (2009)

Semi-transparent Solar Cell

Adv. Mater., 20, 415 (2008)



2008

Anisotropy in Single-Crystal Photovoltaic

Adv. Mater., 20, 435 (2008)

2007

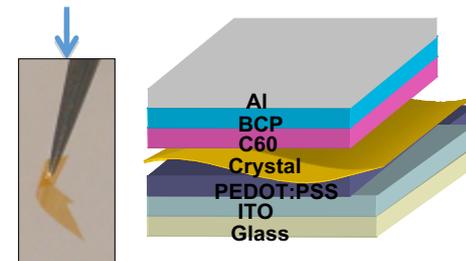
Transition Metal Oxide as Buffer Layer

Appl. Phys. Lett., 88, 073508 (2006), cited 1050 times

2006

Accurate Measurement and Characterization

Adv. Funct. Mater., 16, 2016 (2006)



Solvent Mixture Effect

Adv. Mater., 18, 1783 (2008)

Solvent Annealing Effect

Adv. Funct. Mater., 17, 1636 (2007),
cited 1200 times

Inverted Structure

Appl. Phys. Lett., 88,
253503 (2006)

2005

Controlling of Active Layer Growth Rate (4.4%)

Nat. Mater., 4, 864 (2005), cited 5742 times

2003 (<1%)

Certified World Records: 6.8% → 7.6% → 8.1% → 8.6% → 10.6% → 11.5% → 12.6%

YY Lab: 養成一個課題組的文化，鼓勵學生去尋找突破點。

Example : Project-X (2007)

- 在2007年的時候，我們決定開創 柔性 “無機半導體” 的方向。
- 我挑戰我的課題組，看看有沒有學生願意出來接受這個挑戰。結果有四個學生願意來做這件事情。
- 他們花了一個暑假的時間讀文獻，專利最後我們確定了一個方向：CIGS: 這是一個無機半導體，同時也是柔性半導體。
- 結果4年之後鈣鈦礦太陽能電池的研究開始，我們已經準備好了。



Vincent Tung



William Hou

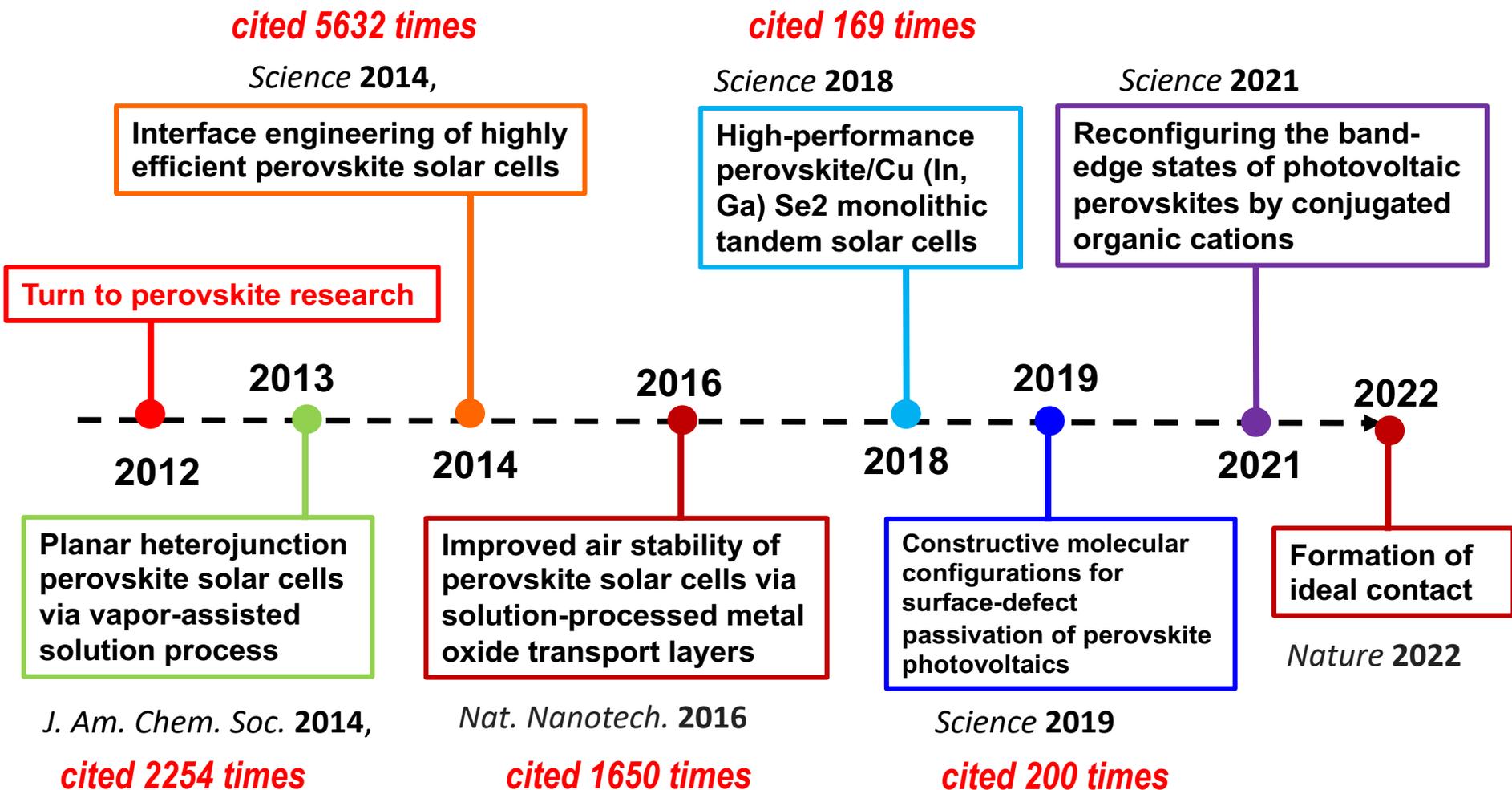


Peter Li



Matt Allen

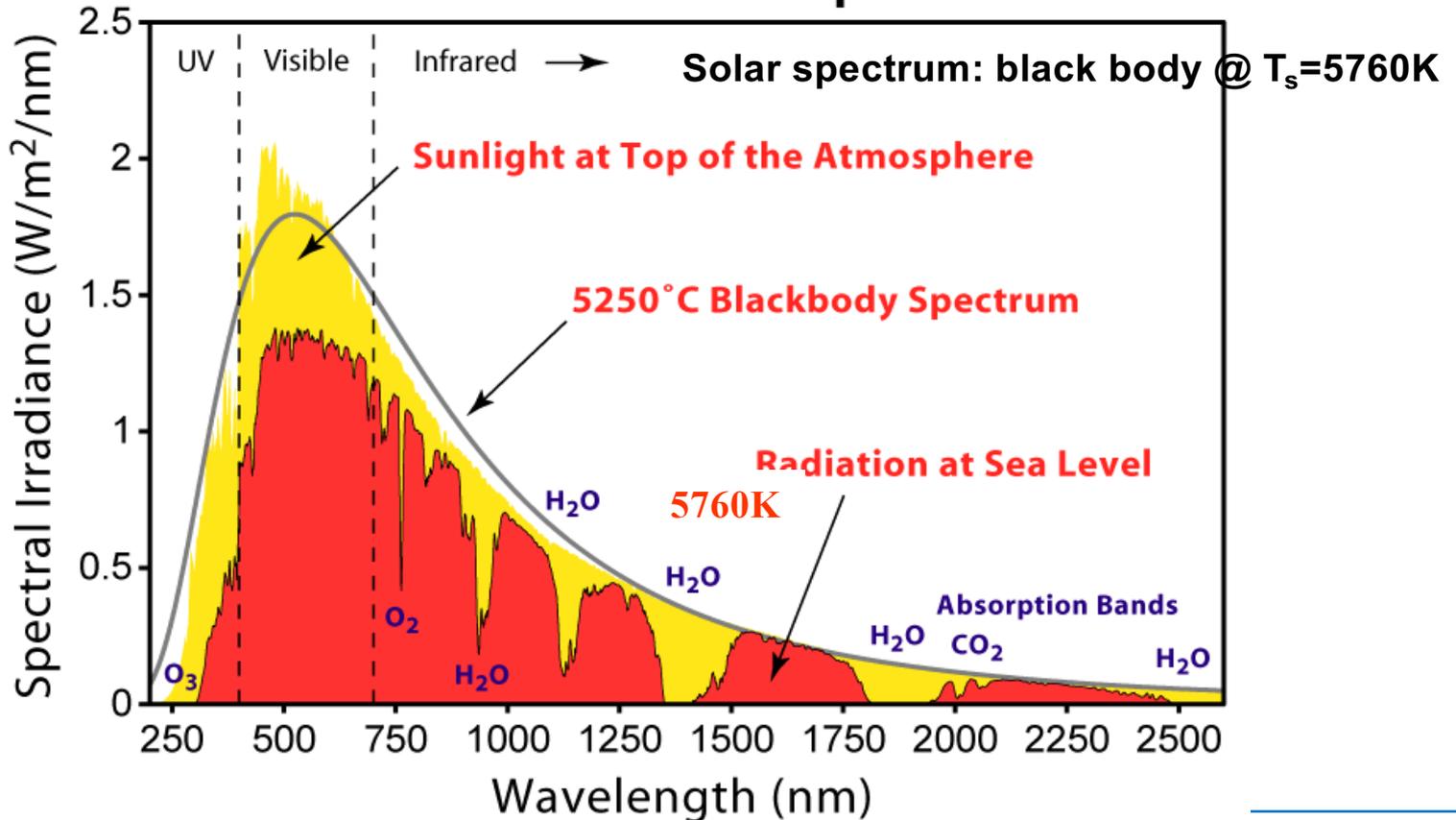
YY Lab PVSK Research Milestones



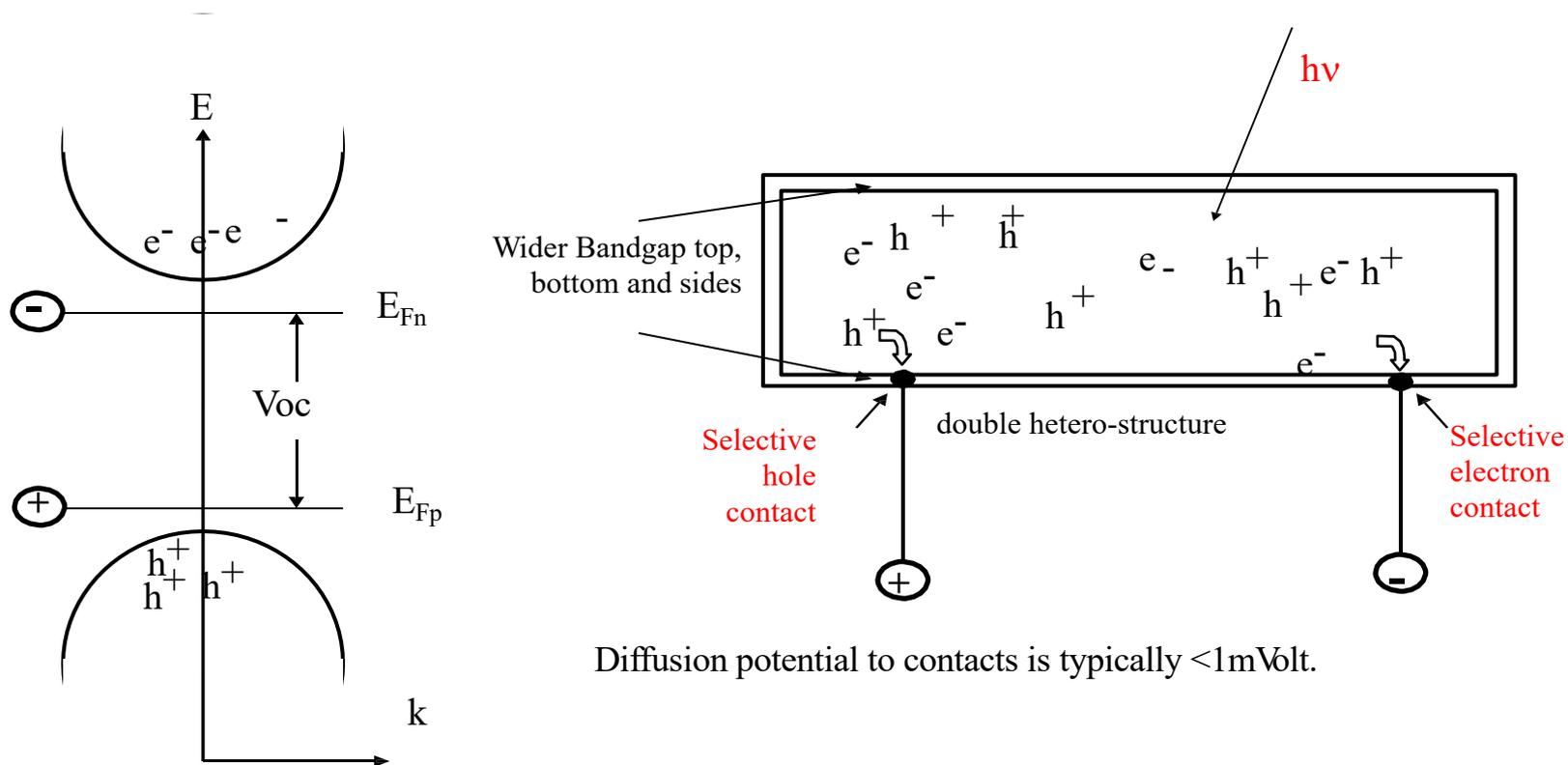
Black Body:

Black body refers to an object or system which absorbs all radiation incident upon it and re-radiates energy which is characteristic of this radiating system only, not dependent upon the type of radiation which is incident upon it.

Solar Radiation Spectrum



A simple model on PV



A good Solar Cell does not require a p-n junction!*

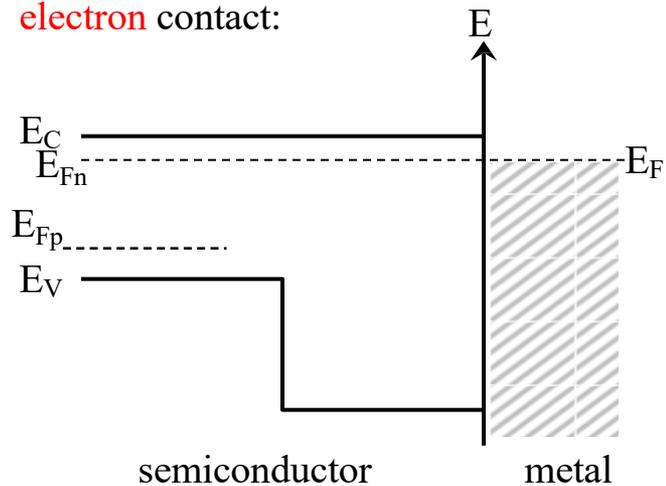
*<http://energyseminar.stanford.edu/node/369>

Courtesy of Prof. Eli Yablonovitch

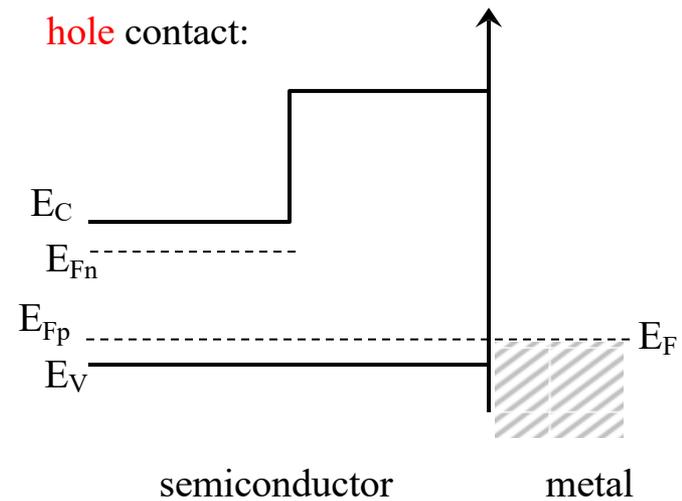
What is a Selective Contact?

It passes one type of carrier but not the other.
The ideal type of selective contact is a hetero-contact:

electron contact:



hole contact:



Courtesy of Prof. Eli Yablonovitch

Better Fundamental Understanding Leads to Breakthroughs



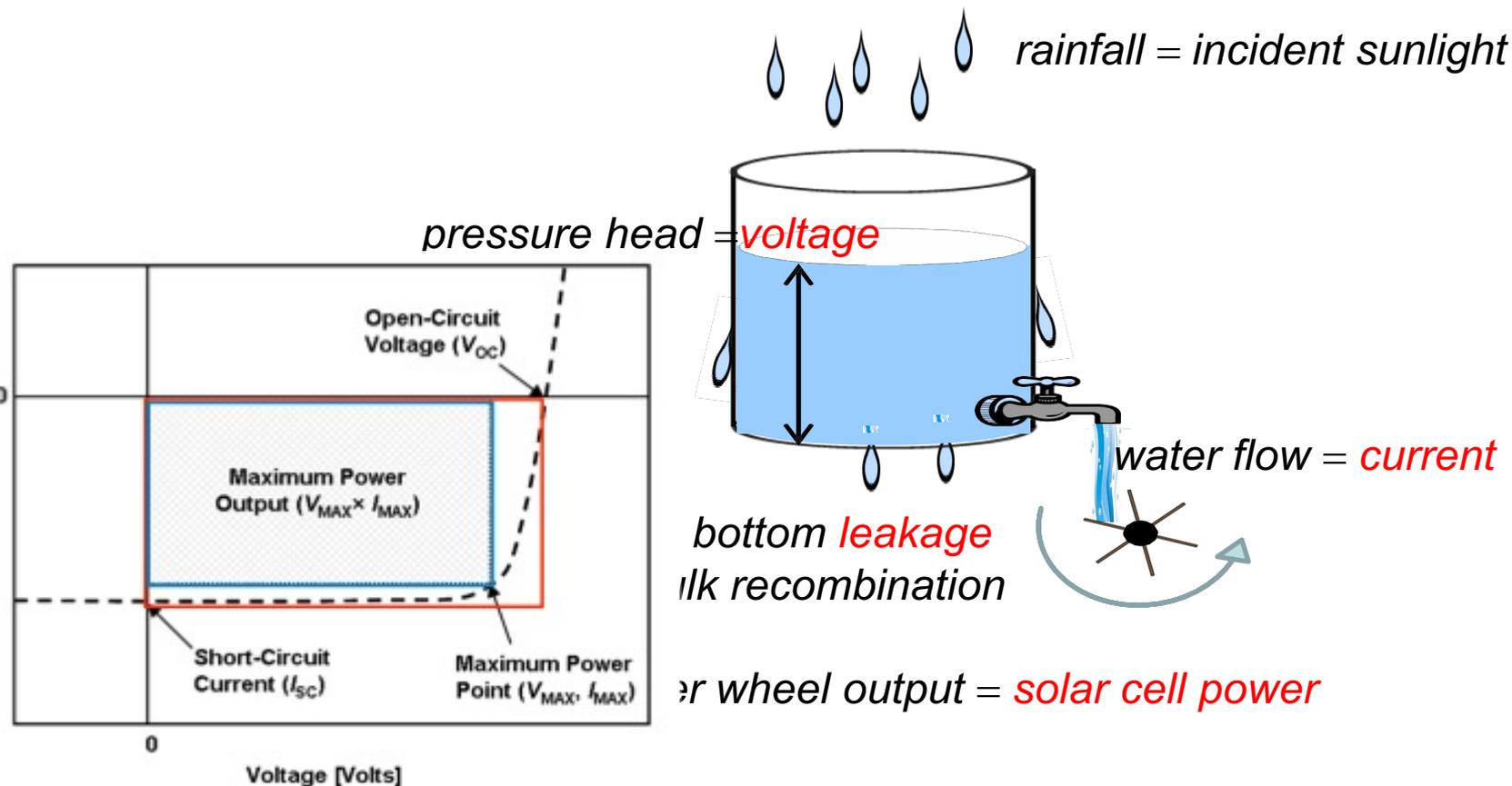
$$V_{oc} = \frac{nkT}{q} \ln\left[\frac{I_{ph} - I_0}{I_0}\right] \approx \frac{nkT}{q} \ln\left(\frac{I_{ph}}{I_0}\right)$$

Eli proposed:

$$qV_{oc} = qV_{oc,max} - kT|\ln \eta_{ext}|$$

$V_{oc,max}$ is the maximum V_{oc} that can be extracted

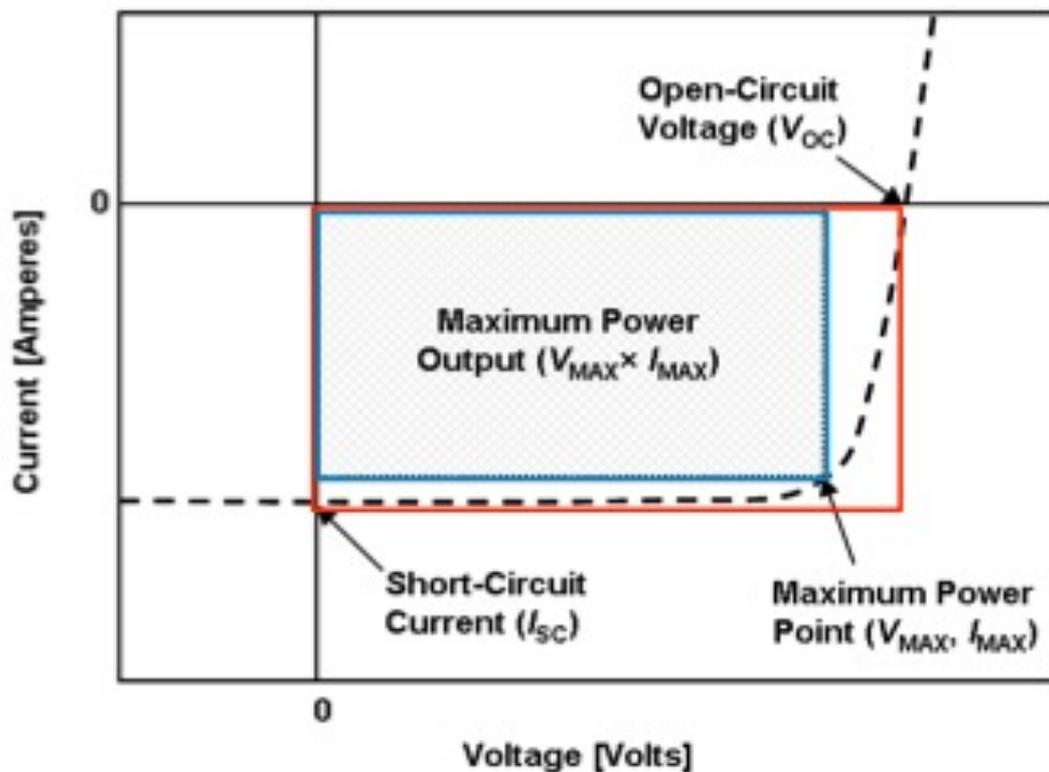
η_{ext} is external PL quantum efficiency



$$PCE = J_{sc} \times V_{oc} \times FF$$

Courtesy of Prof. Eli Yablonovitch

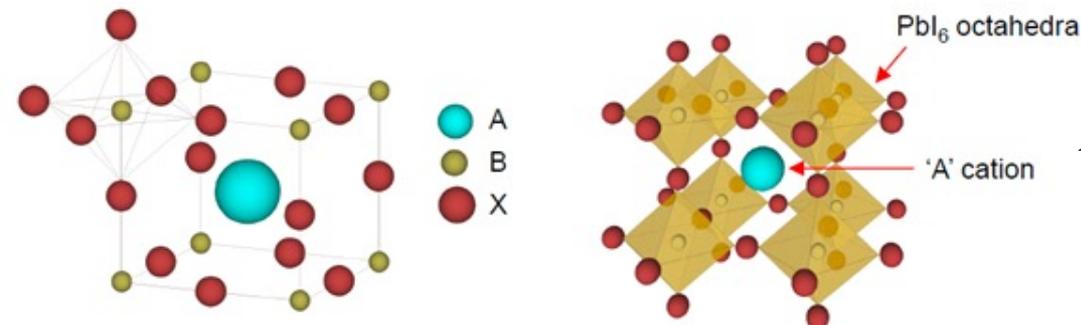
Power Conversion Efficiency



$$PCE = J_{sc} \times V_{oc} \times FF$$

Metal-halide perovskite solar cells: introduction

- Metal-halide perovskite: An ideal material for photovoltaic



A = CH_3NH_3^+ (MA^+), $\text{HC}(\text{NH}_2)_2^+$ (FA^+), Cs^+

B = Pb^{2+} ,

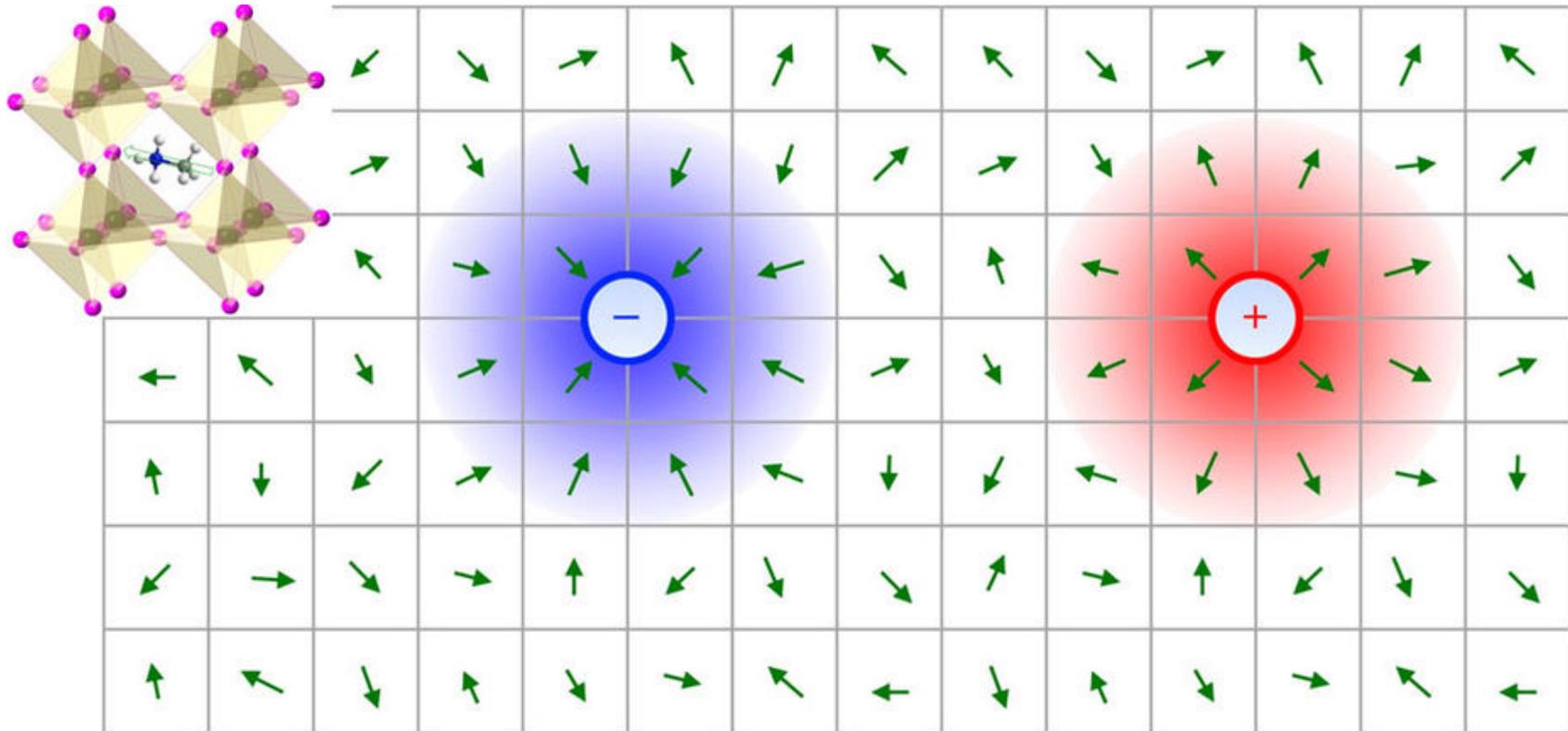
X = Cl^- , Br^- , I^-



Advantages:

- ✓ Long-range charge carrier diffusion lengths
- ✓ High defect tolerance
- ✓ Strong absorption
- ✓ Simple processing

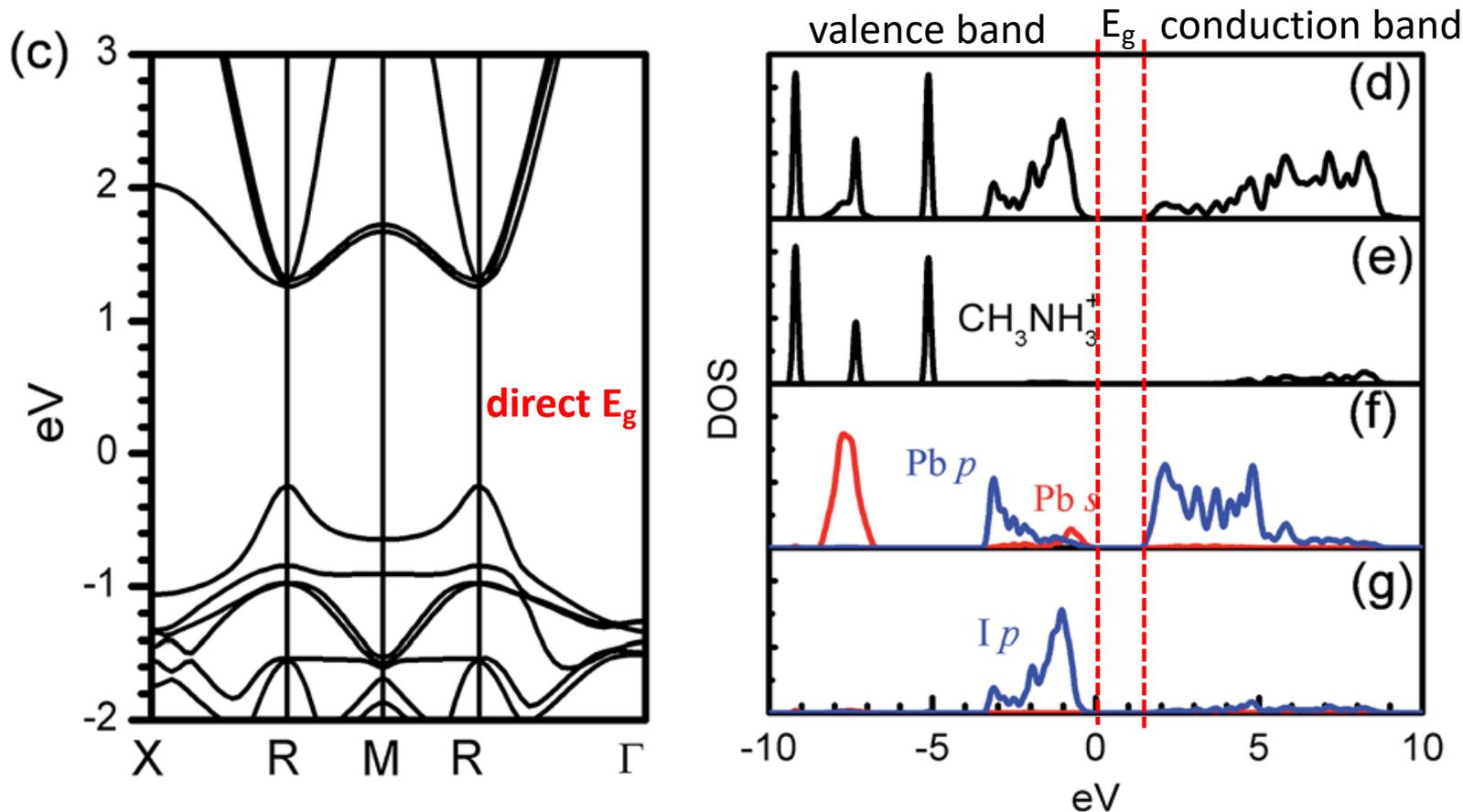
	Perovskite	Si	CIGS	GaAs
Band gap (eV)	1.5 (tunable)	1.1	1.12	1.43
Absorption coefficient	10^4 - 5	10^3	10^4 - 5	10^4 - 5
Carrier mobility $\text{cm}^2/(\text{V}\cdot\text{s})$	Up to 2000	1500	< 10	8500
Carrier lifetime	> 100 ns	ms	50-200 ns	<100 ns



→ Large polaron effect enables *extremely long carrier lifetime* comparable to that of high-purity inorganic semiconductors such as GaAs.

[1] X.-Y. Zhu et al. *Sci. Adv.* **2017**, 3, e1701217.

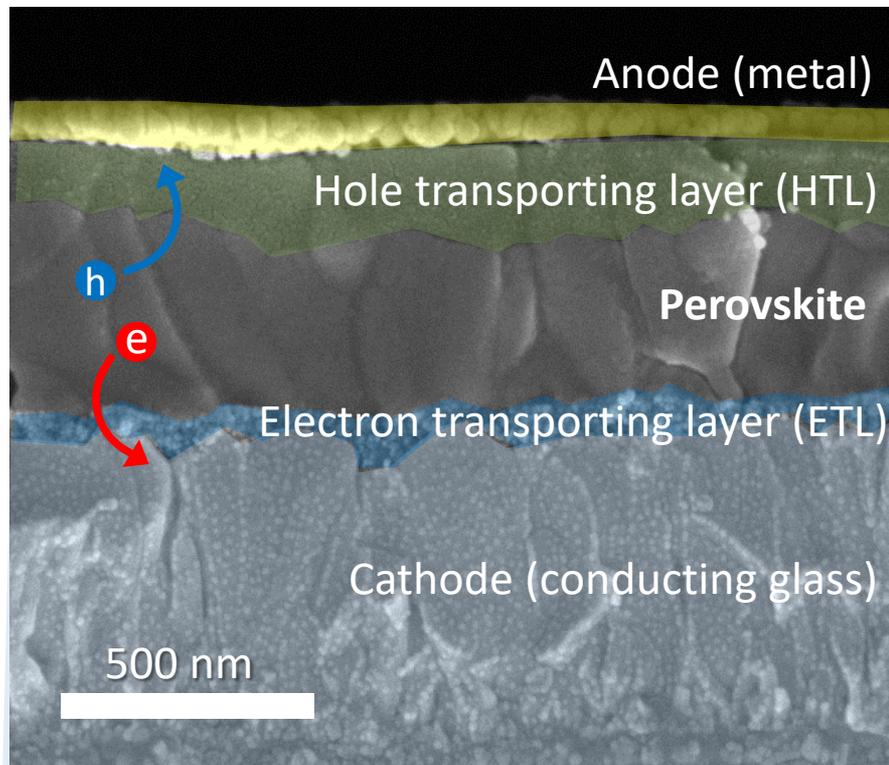
[2] V. Podzorov et al. *Nat. Commun.* **2016**, 7, 12253.



- Valence band maximum (VBM) : from I p and Pb s orbitals
- Conduction band minimum (CBM) : from Pb p orbital
- A cation does not directly contribute to VBM and CBM

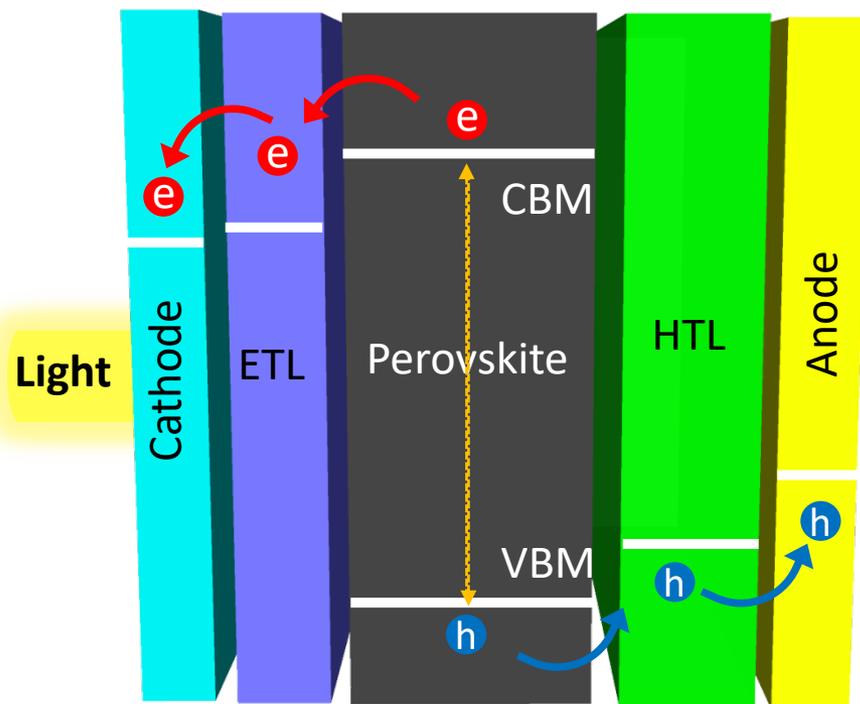
Introduction: perovskite solar cells

Device structure (SEM image)



Light

Energy band diagram

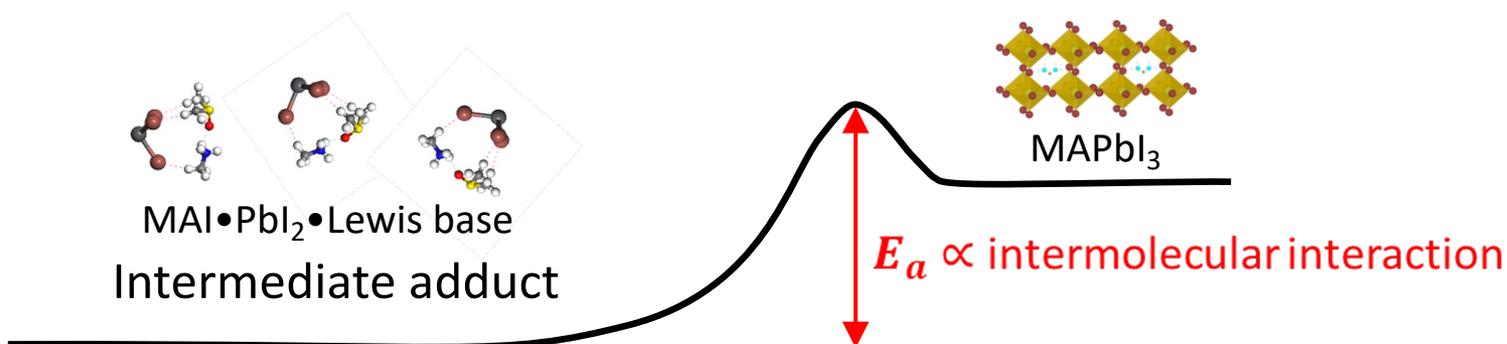


Kinetics control for enhanced crystallinity

Classical crystal growth theory:

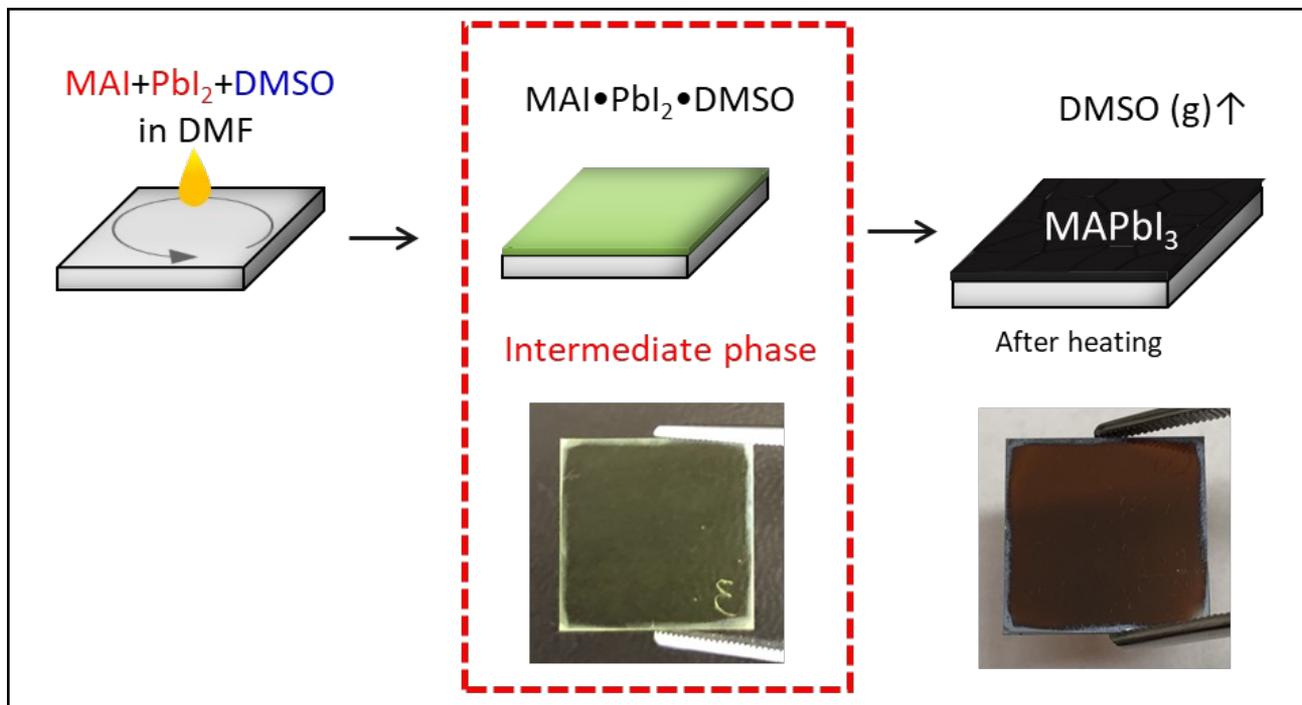
$$\frac{dN}{dt} = A \exp\left(-\frac{E_a}{k_B T}\right)$$

*Tune the activation energy to slow down
the crystallization process*



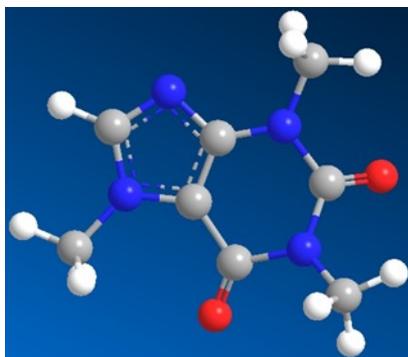
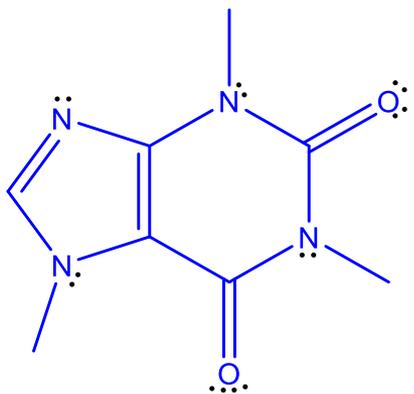
Intermediate adduct phase is used to control the crystallization kinetics

- Control the crystallization process

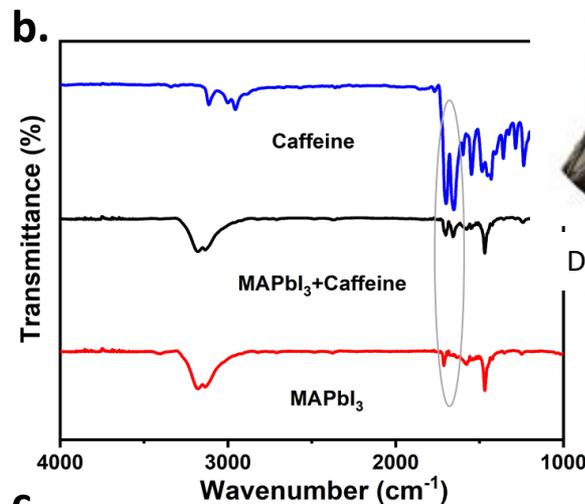


Caffeine: formation of adduct

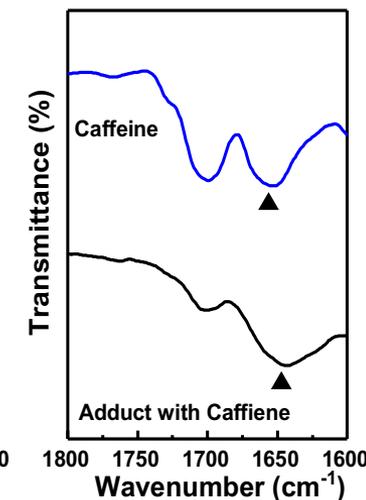
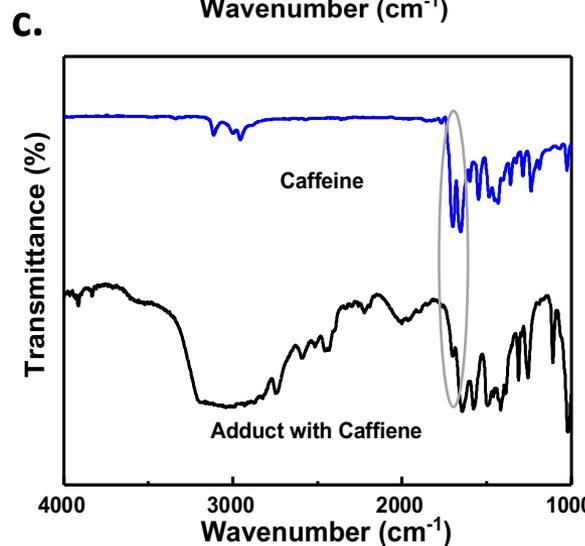
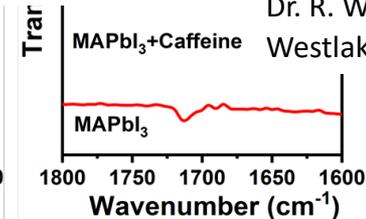
Molecular structure of caffeine



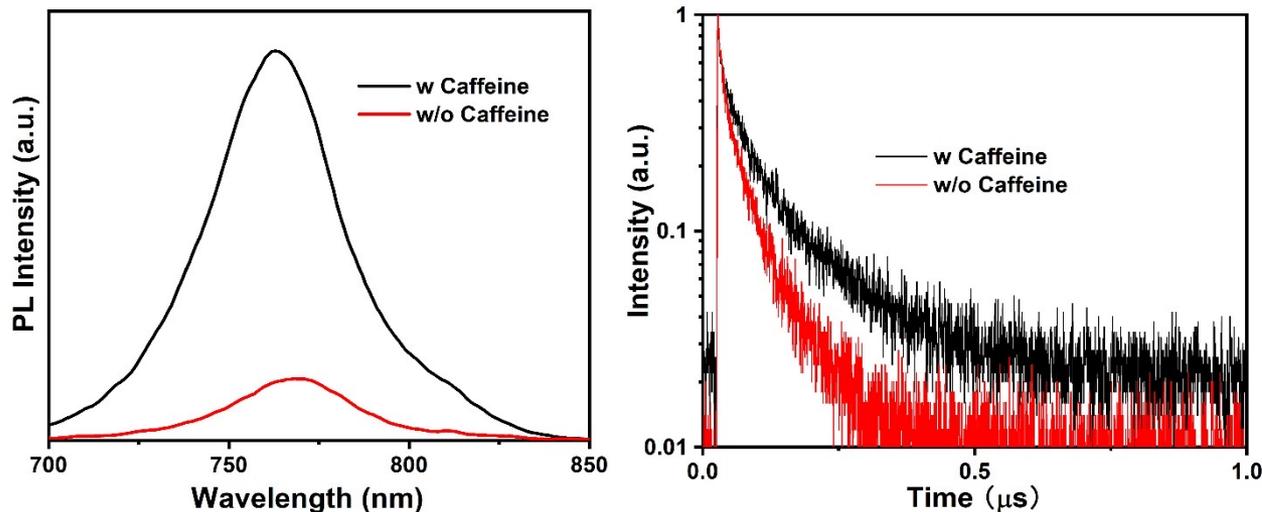
Interaction between C=O in



Dr. JJ Xue, ZJU

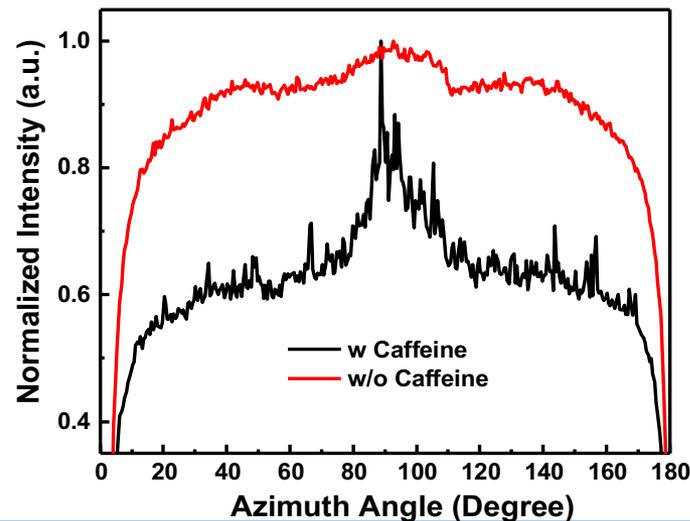
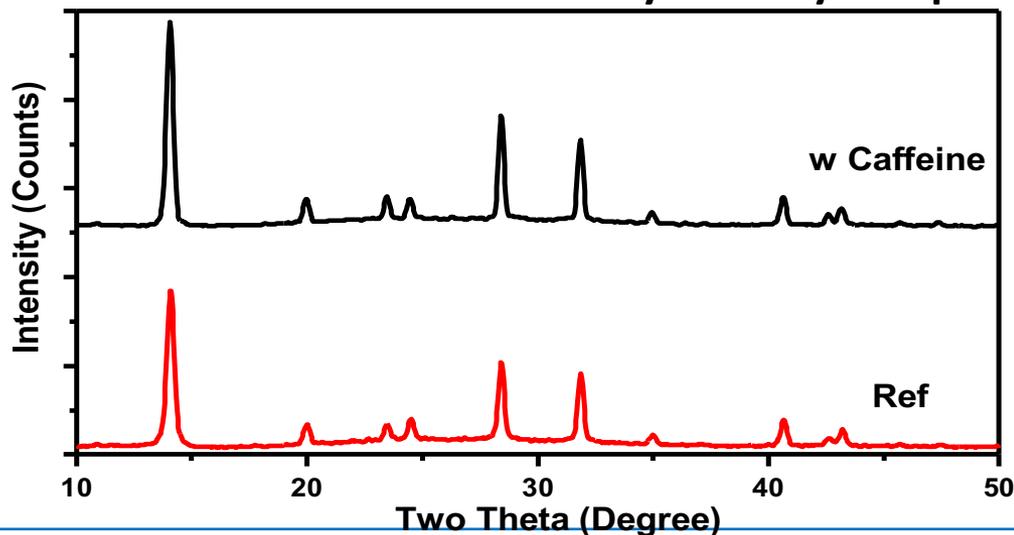
Dr. R. Wang
Westlake U.

Perovskite thin film properties

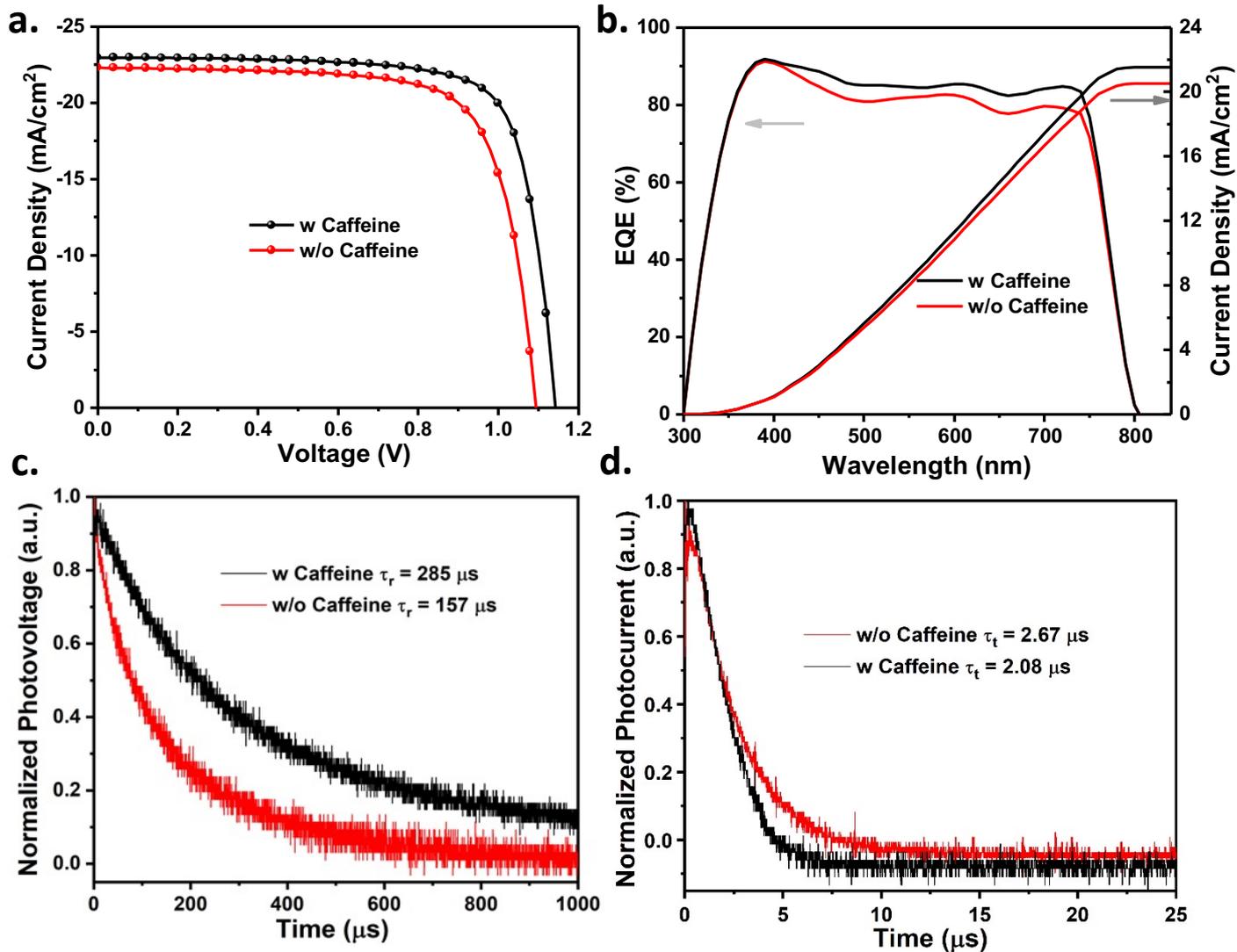


Enhanced photoluminescence (PL) and PL lifetime

Enhanced crystallinity and preferred crystal orientation

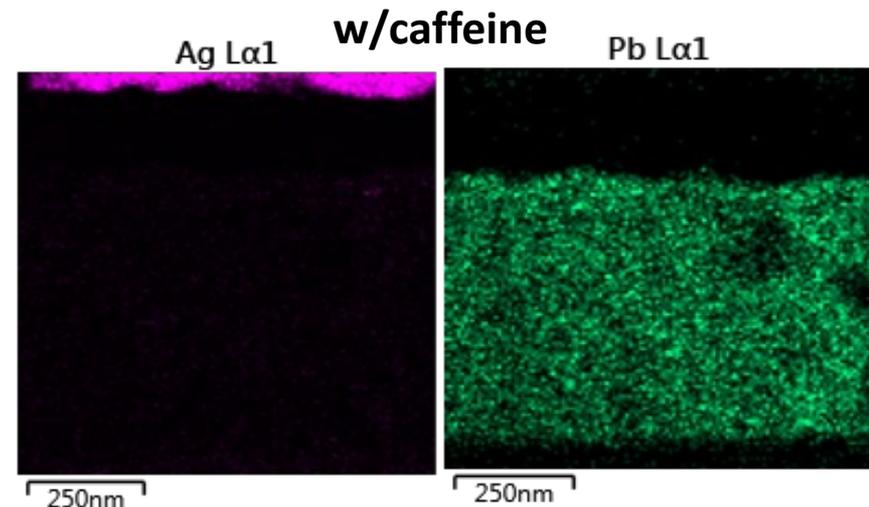
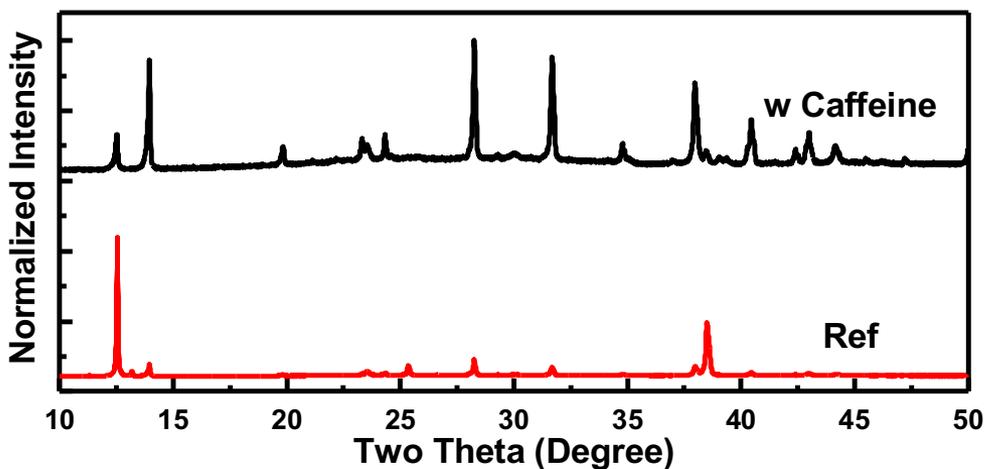
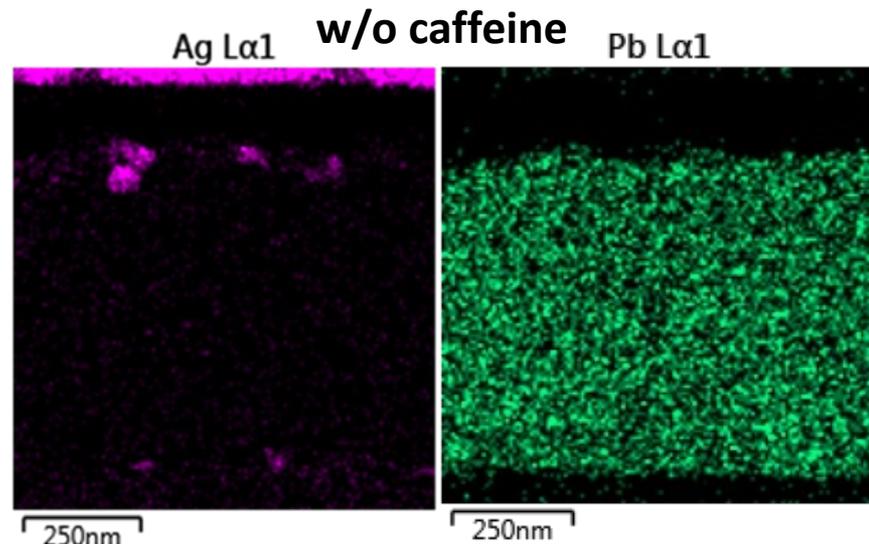
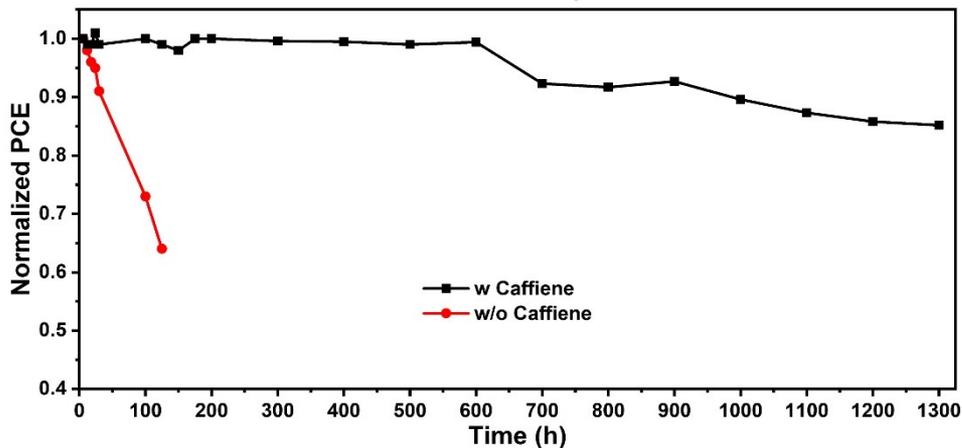


Device performance and carrier dynamics



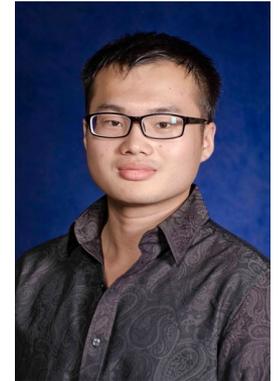
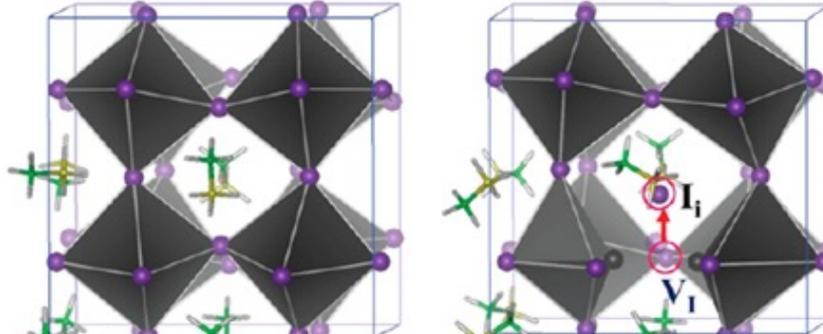
Improved thermal stability

1300 h at 85°C (NIP, PTAA as HTL)



[1] Rui Wang and Y. Yang et al. *Joule*, 2019.

- Cations: effective additives to improve operational stability of perovskite solar cells



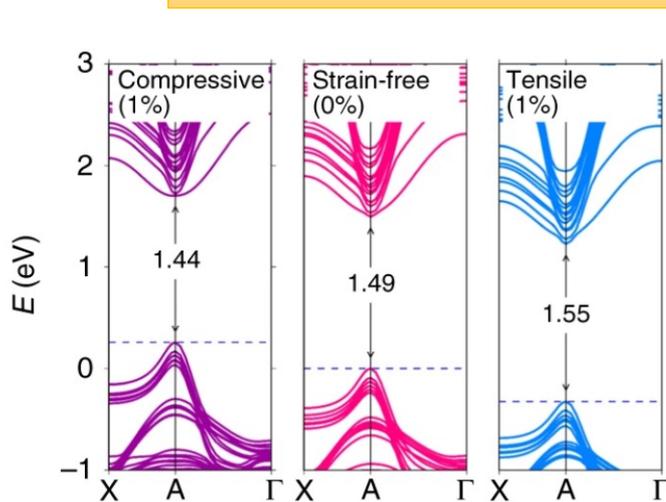
Dr. YP Zhao, UCLA

Hence, it is important to find out an efficient interstitial doping

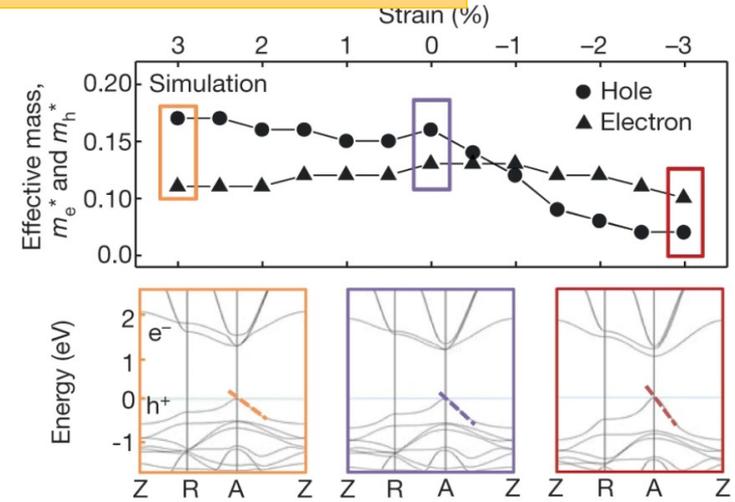
- However, the **text**

140(4): 1358-1364 (2018)

basic performances

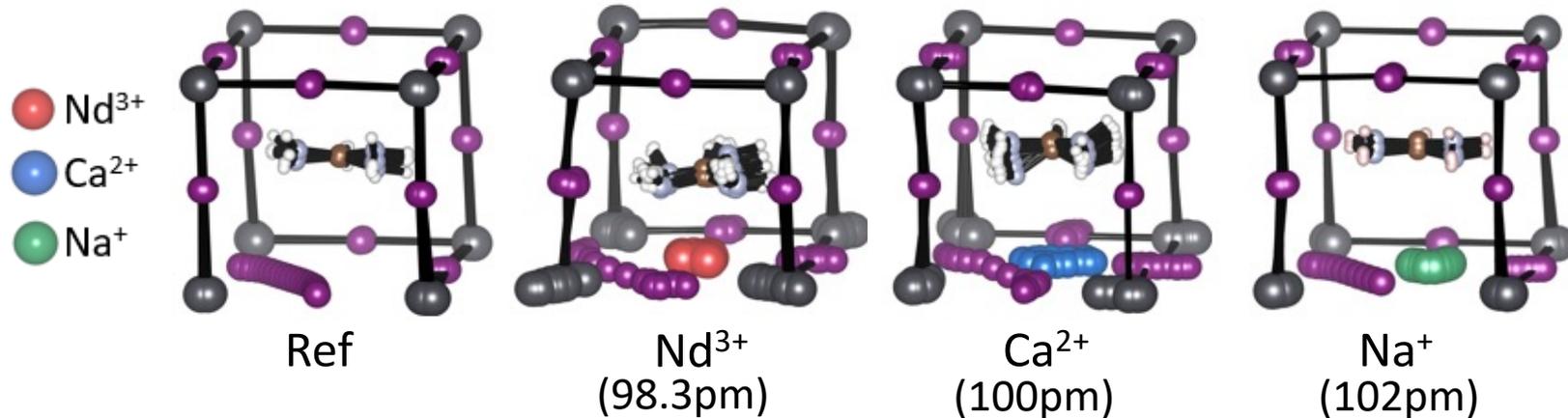


J. Huang et al. *Sci. Adv.* 3, eaao5616 (2017)

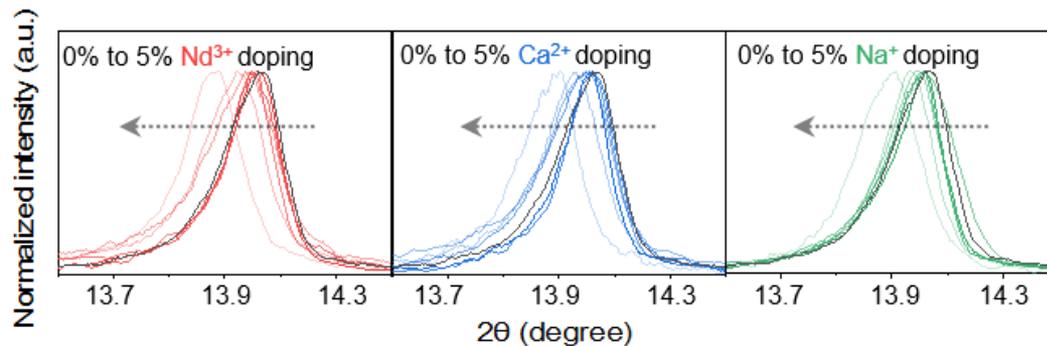


S. Xu et al. *Nature* 577, 209–215 (2020)

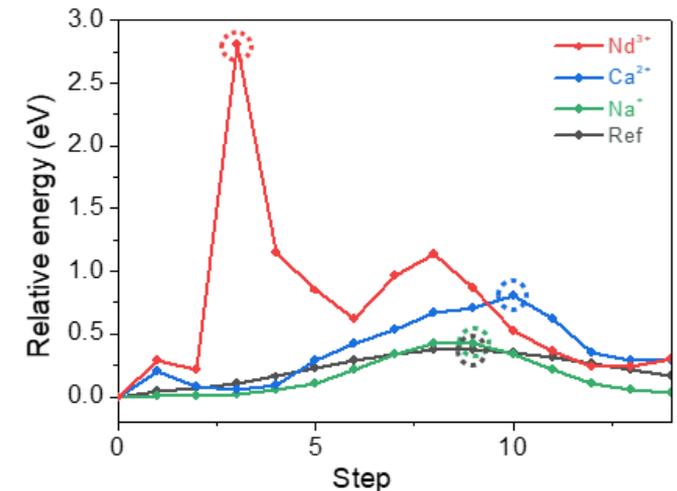
- Start from a well-utilized cation, Na^+ , we compare the interstitial doping ions with similar sizes:



- Confirmed tensile strain introduced by the cations:

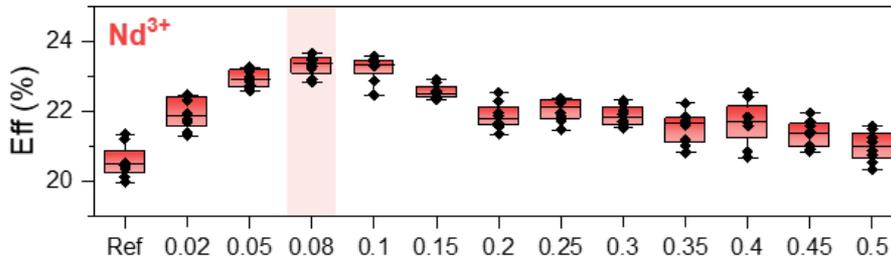


- Relative energy on iodide ion migration pathway:

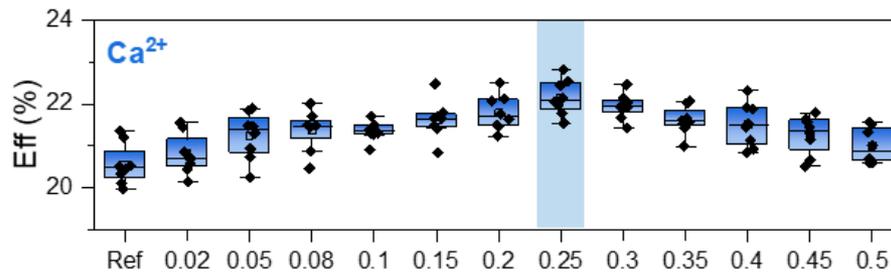


- Less doping amount needed to reach the best performances of the devices with Nd^{3+} :

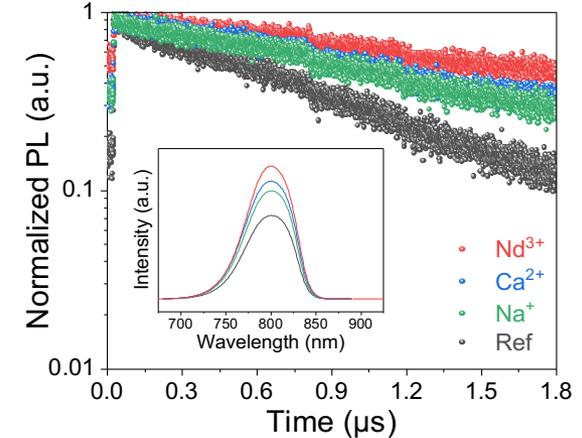
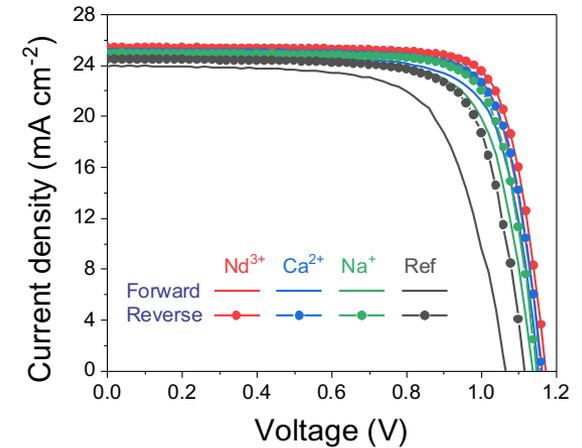
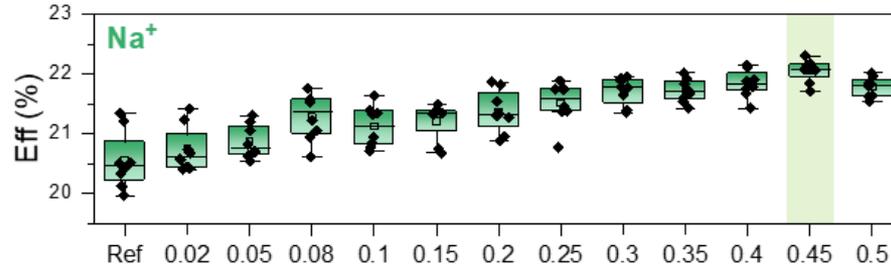
Neodymium
ionic radii:
98.3 pm



Calcium
ionic radii:
100 pm

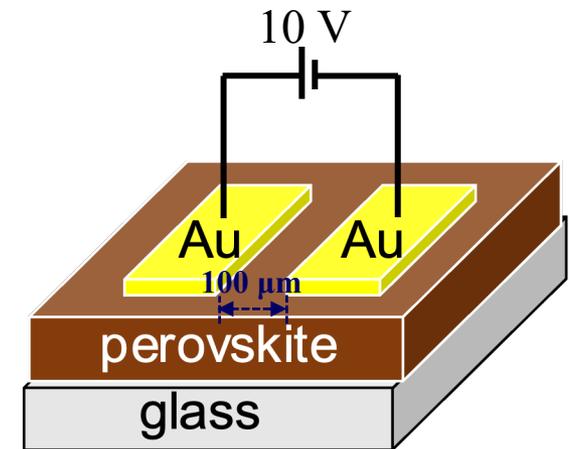
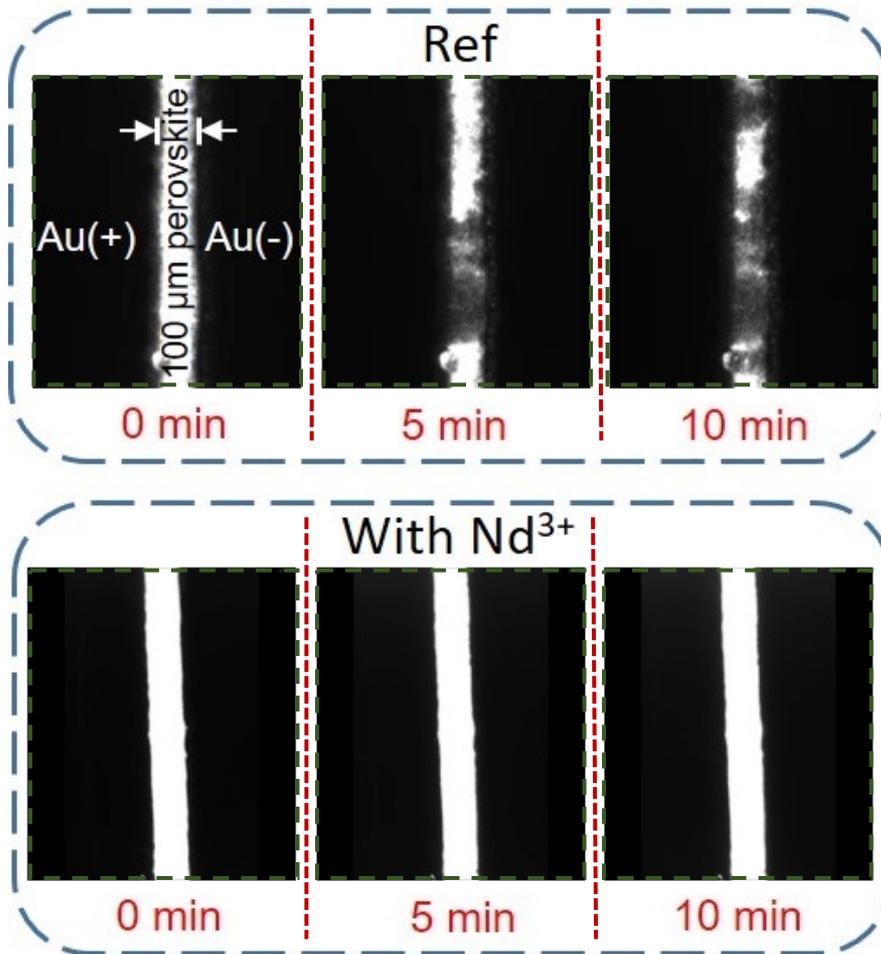


Sodium
ionic radii:
102 pm



In-situ photoluminescence of the lateral devices

- Suppressed ion migration with Nd^{3+} interstitial doping:
In-situ photoluminescence of the lateral devices



- Suppressed ion migration with Nd³⁺ interstitial doping:

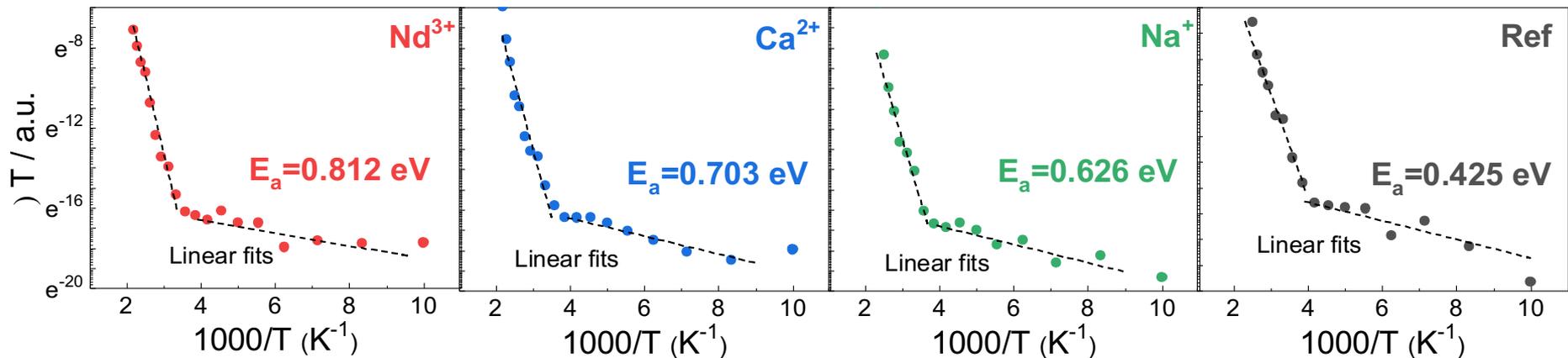
Temperature-dependent conductivity

Nernst–Einstein equation:

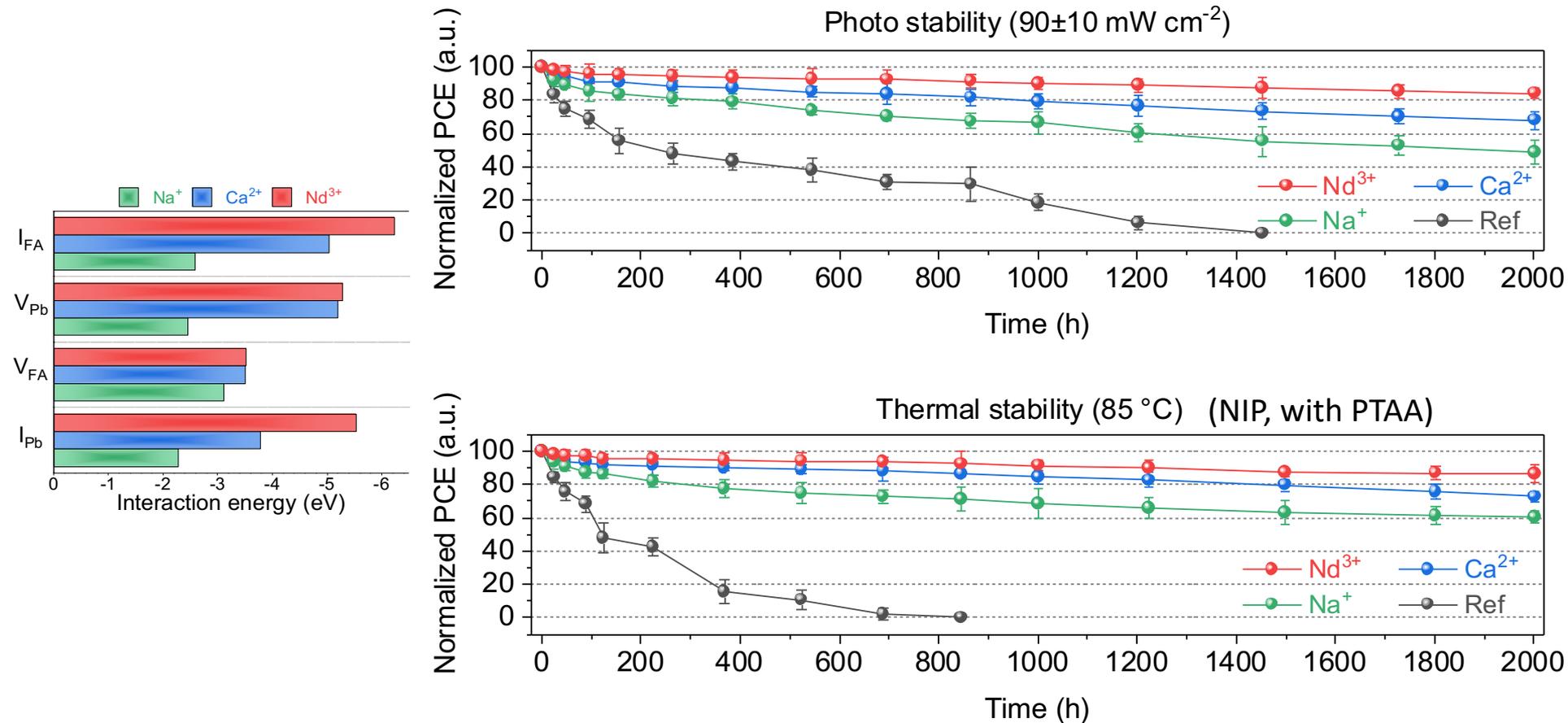
$$\sigma(T) = \frac{\sigma_0}{T} \exp\left(\frac{-E_a}{k_b T}\right)$$

E_a is activation energy; $\sigma(T)$ is the conductivity as a function of temperature T .

E_a for ion migration was extracted from the slope of the fitted lines at relatively higher temperature.



- Elongated device lifetime with Nd^{3+} interstitial doping:



3+1 個故事

一個人的選擇, 往往要數年之後才知道結果 ;

But rather than to worry about did one make a right decision or not,
We should develop a skill of re-build ourselves.

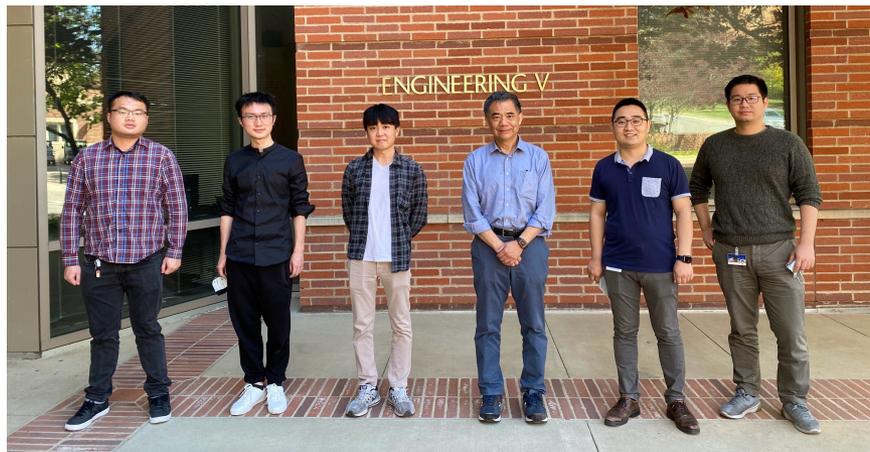
The right logic thinking and good habits
can always guide one to the right direction.

走錯了，怎麼辦？



西湖大學工學院創院院長
2019-2020

2021



YY Lab in 2018





July 2019 – October 2020,
I took a Leave of Absence to join the
Westlake University in China
for a reform of the high-level education.

Returned to UCLA in Oct. 2020



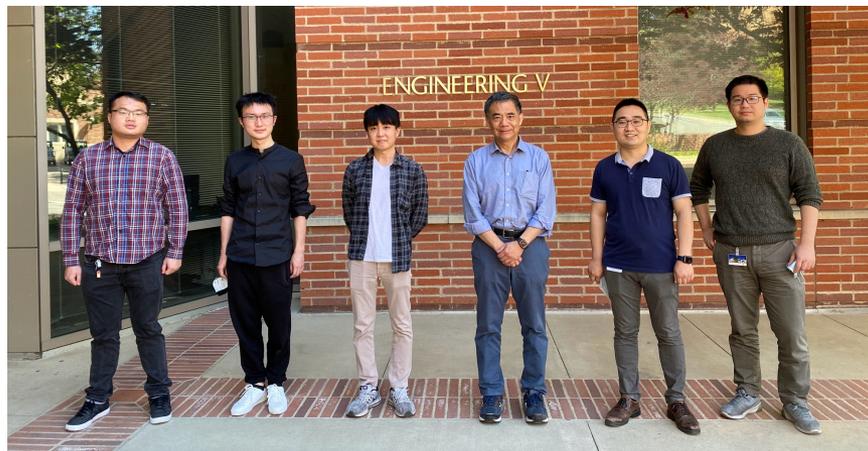
我的西湖工學院經歷 - 西湖大學的兩年半的投入, 可能是我人生中最專註的事情



- **The cornerstone:** Honesty and Integrity;
(誠實和正直, 工學院的基石)
- **Find the best people;** 找最好的人才
- **Let them play:** MRIC (交叉學科中心), so let the PIs have fun to pursue the “impossible”.
- Plus the **winner’s logic.** 贏家的邏輯思維



2021



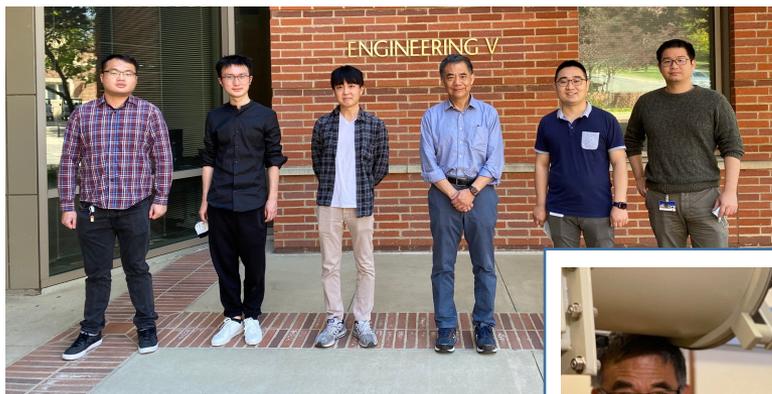
怎麼辦?

I don't want to repeat myself, so, I must reinvent the future.

The YY Lab has been UCLA born.



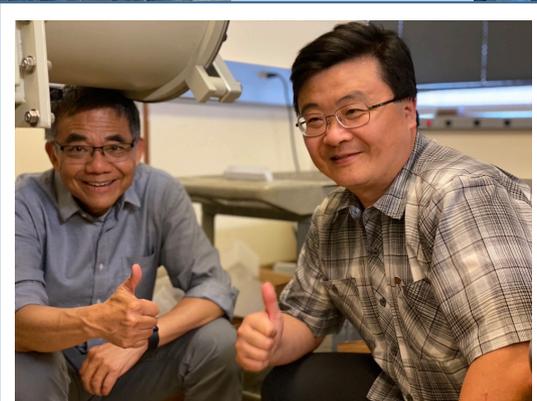
- Our group had only five people remaining.
- We need to re-build the YY Lab.
- Our Y6 molecule was missing.



August 2022



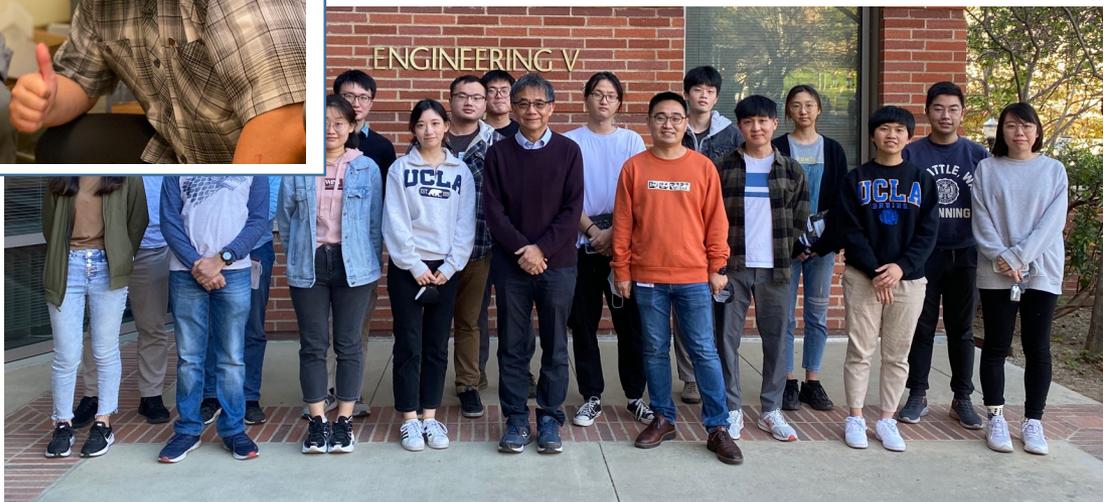
and the teamwork.



Fall 2021



Summer 2022



We re-built the team,

12/11/22

Competition is the key to success



- 今天我有一個想法， **let us compete!**
- Because we can only connect the dots backwards;
- 所以我今天想跟各位提一個建議，讓我們從現在開始以未來三年或者是五年的時間，我們來回顧我們的成就。
- **Rule 1:** we back in **three years** and let the committee to evaluate this group of young faculty and YY's achievements. (**三年之後, 阿里山論劍**)。
- **Rule 2:** 排資論輩，敬老尊賢，這個都不予考慮。
- **Rule 3:** YY 不得以他現有的光伏研究來充數。

事實上年輕教授占很大便宜

- 精力 VS 經驗
- 激情 VS 夕陽
- 有錢 VS 沒錢
- 壓力 VS 退路

賭不賭?

