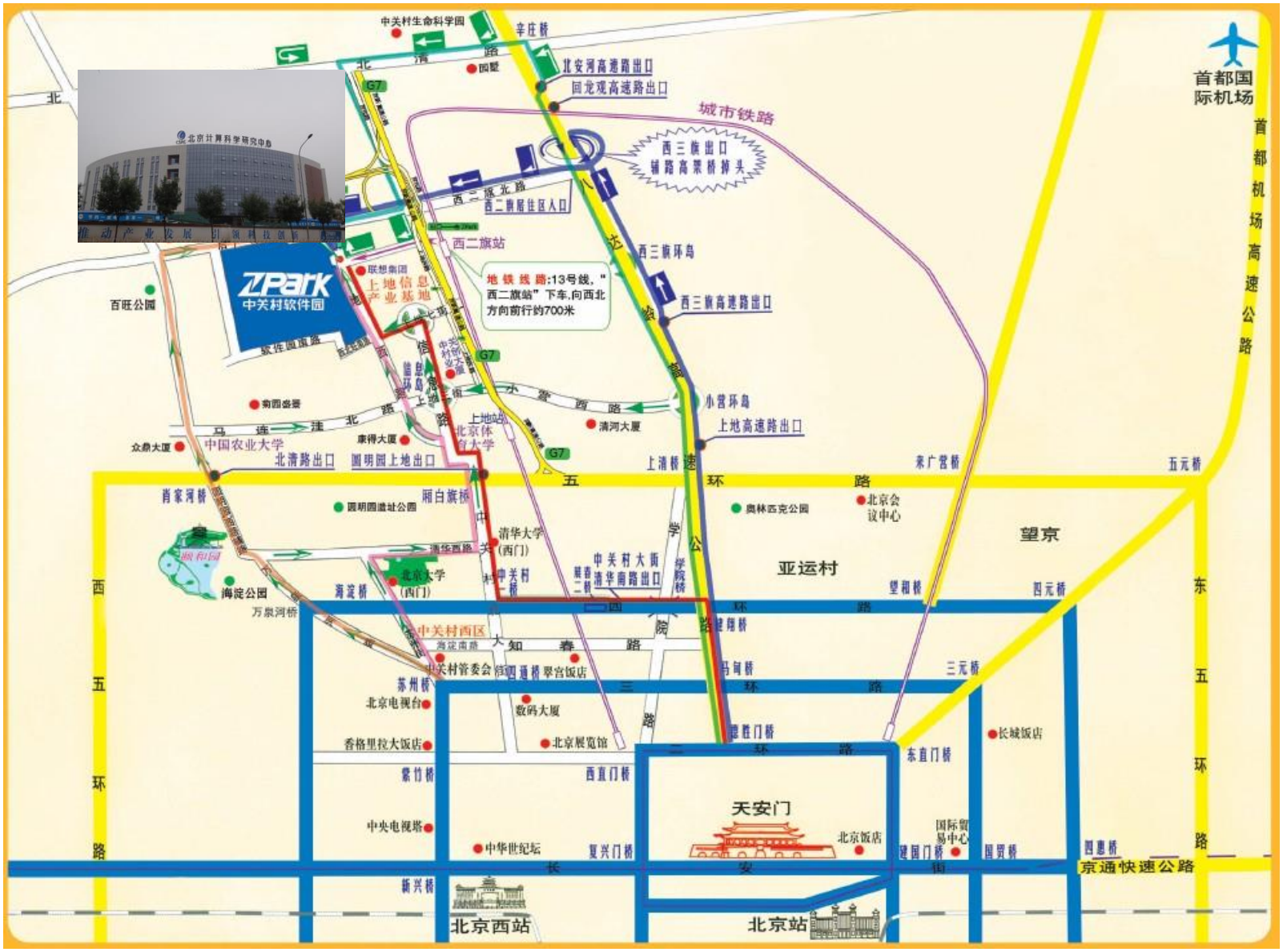
First Principles Design of Materials for Energy and Optoelectronic Device Applications

Su-Huai Wei

Beijing Computational Science Research Center

CSRC

CSRC Location: ZPark



CSRC

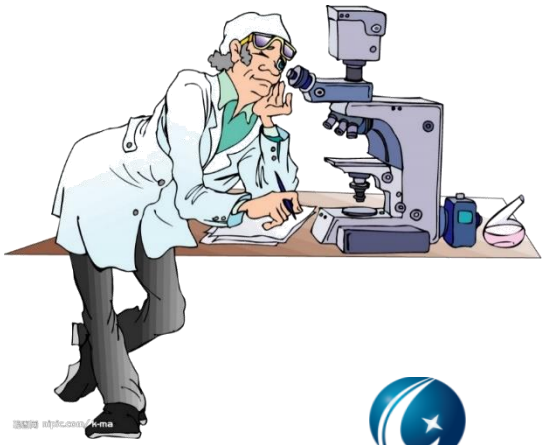
- Beijing Computational Science Research Center (CSRC) was founded in 2009 and it is an interdisciplinary fundamental research organization focusing on computational study.

- Conduct basic and frontier research; attract talents worldwide; promote international academic exchange and collaboration.

Research Laboratories

The Center has recruited senior and young scientists worldwide to do interdisciplinary and innovative researches, and currently it has established 7 divisions：

- Quantum Physics and Quantum Information Division
- Physical Systems Simulation Division
- Materials and Energy Division
- Complex System Division
- Applied Mathematics Division
- Mechanics Division
- Algorithm and Computer Science Division



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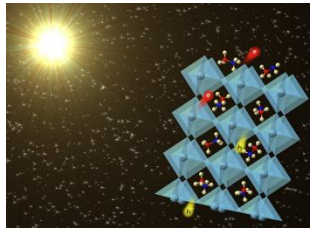
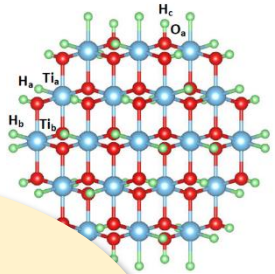
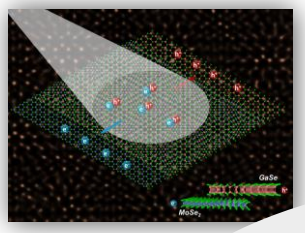
Research Activity of Material and Energy Division







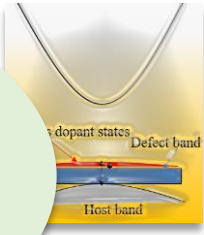
PV Materials:
Explain the underlying physics of new experimental observations; Design new PV materials with high efficiency and low cost

Catalytic Materials:
Develop materials for H_2 production through PEC water splitting. Find materials that can use solar energy and CO_2 reduction to generate fuel.

Nano Materials:
Design low-dimensional systems for energy applications.
Develop advanced theoretical approaches for these quantum materials.

Material Design For Energy Applications

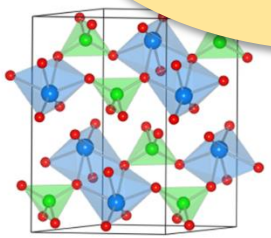
Theory of Doping in Semiconductors:
Develop new physics of doping theory; provide new strategies to overcome the doping bottlenecks; alter physical properties of a materials through defect control

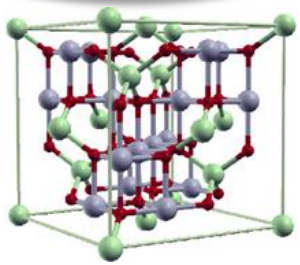


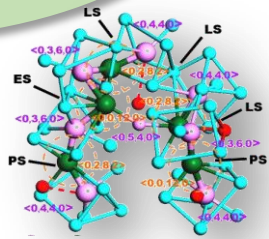
Inverse Design of Novel Materials:
Develop new techniques to predict material properties and design materials with prescribed physical properties

Energy Storage Materials:
Understand and design new materials for battery, supercapacitor, hydrogen and thermal storage applications

Amorphous Materials
Understand the nature of glass and glass transition for high performance amorphous materials





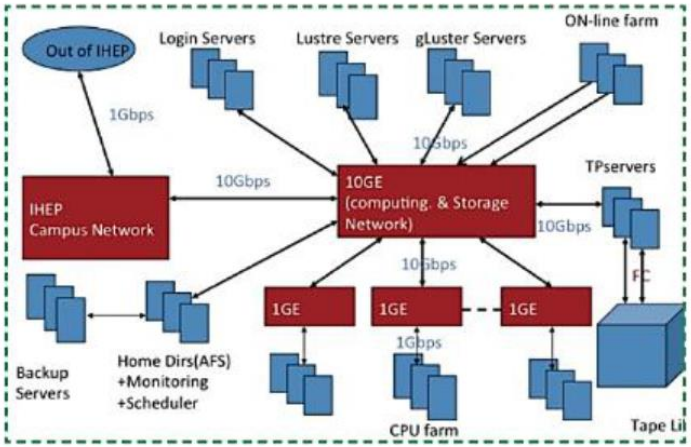


Excellent Research Environment

14112cores

131.1TB Memory

1440TB disks
2304TB back-up disks



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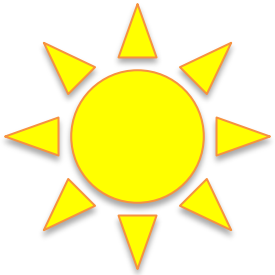
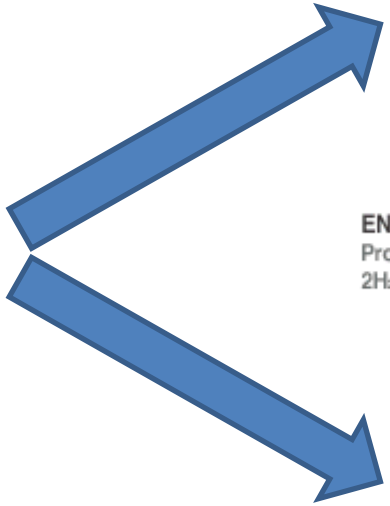
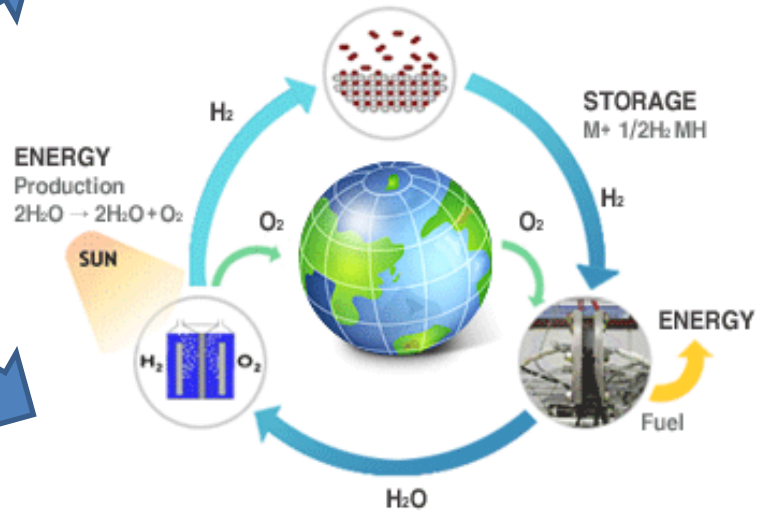
Developing Clean Solar Energy Is Important for Energy Security and Environment



Solar Electricity





Solar Fuel

Fossil fuel is limited and can cause environmental problem. They should be replaced by clean energy such as solar energy.

Computational Design

- Clean energy applications require new functional materials with unique structural, optical, electrical, and thermo properties

- Recent development in first-principle theory and computational power has made *ab initio* knowledge-based material design possible

- First-principles design of functional materials has now become a vital tool for accelerating scientific discovery of clean energy materials

First-Principles Calculation of Material Properties

- Total energy, structural parameters, elastic constants, stress, force, phase stability, phonon spectrum, thermal properties
- Band structure, electron energy levels, density of states, optical transition coefficient
- Charge density distribution, electric field gradient, transport coefficient, diffusion coefficient
- Magnetic moment, spin density, hyperfine interaction parameters, magnetic coupling strength

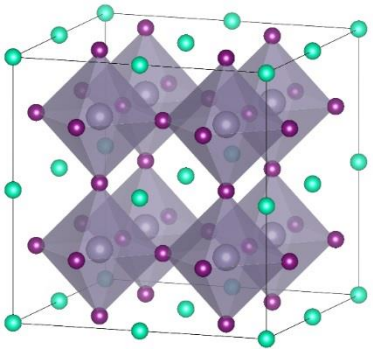
➢ Select materials with targeted material properties for specific energy related applications.

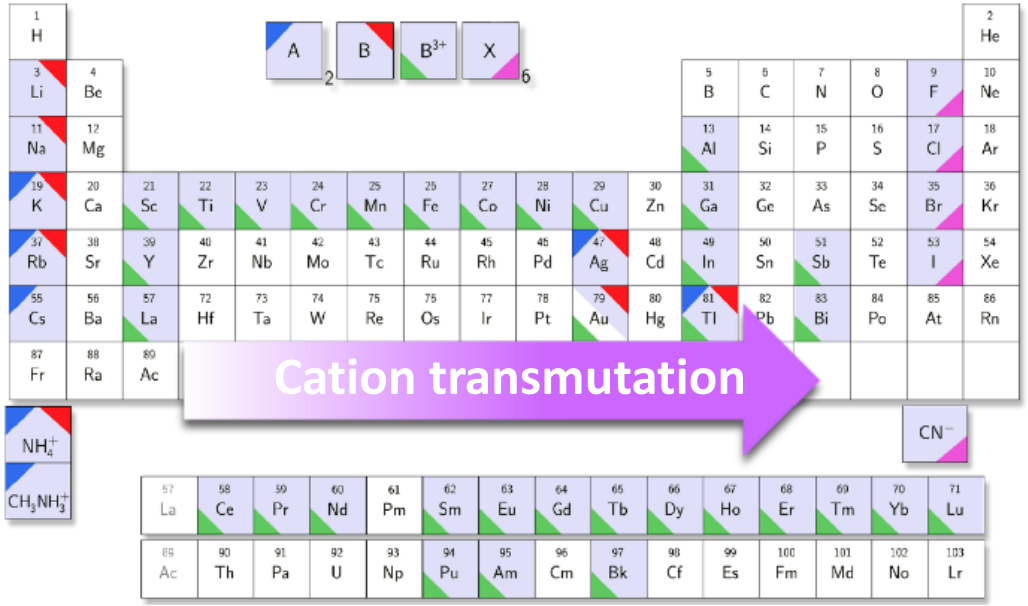
Outline

- Design Stable and Lead-free Inorganic Perovskite Solar Cell Absorbers
- Design Oxides for Hydrogen Production through PEC Water Splitting
- Develop Bipolarly Dopable Transparent Conducting Materials
- Understand the Origin of the Self-limited Energy Density of Cathode Materials for Li-ion Batteries

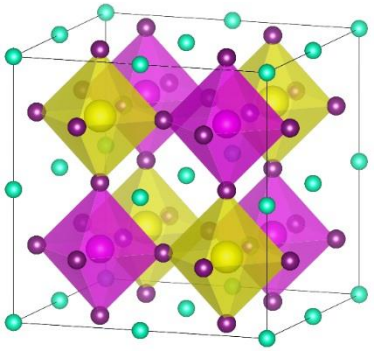
Design Stable and Lead-free Inorganic Perovskite Solar Cell Absorbers

Perovskite





Double perovskite

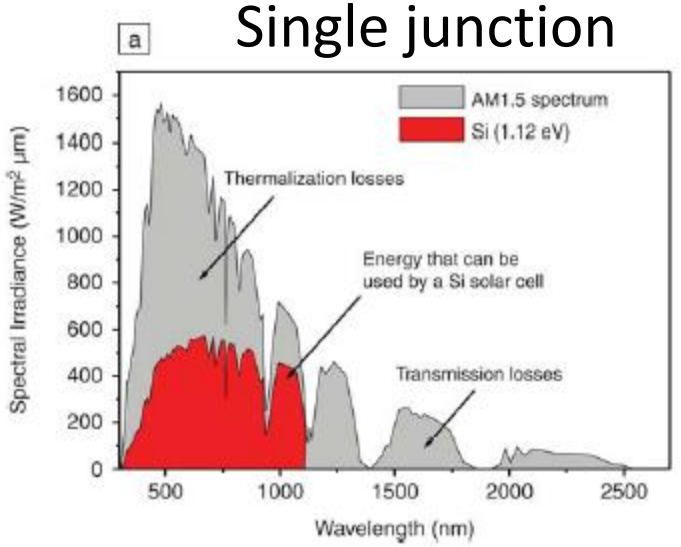


"Halide perovskite materials for solar cells: A theoretical review", W.-J. Yin, J. Yang, J. Kang, Y. Yan, and **S.-H. Wei***, J. Phys. Chem. A **3**, 8926 (2015);

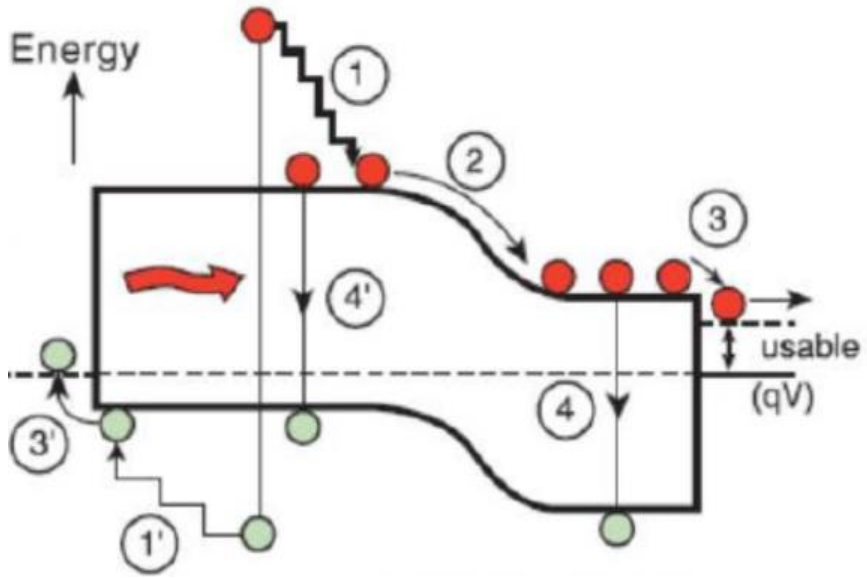
"Design of lead-free inorganic halide perovskites for solar cells via cation-transmutation", X. Zhao, J.-H. Yang, Y. Fu, D. Yang, Q. Xu, L. Yu, **S.-H. Wei*** and L. Zhang*, J. Am. Chem. Soc. **139**, 2630 (2017).

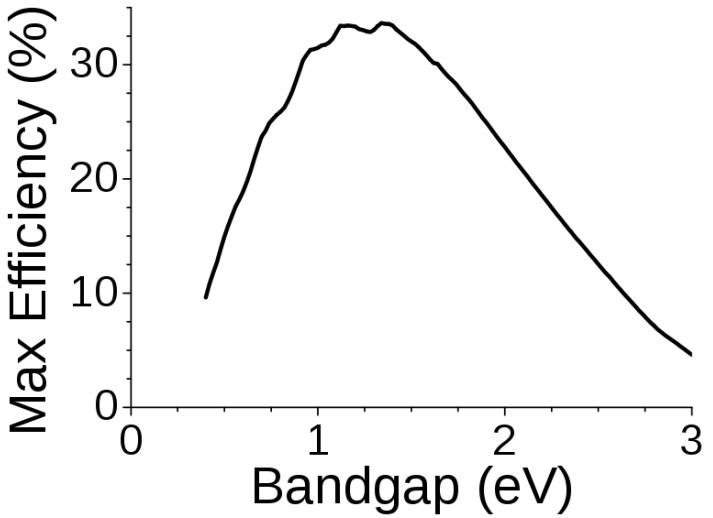
Requirements for Single Junction Solar Cell Absorbers

Single junction



- Optimal direct band gap 1.0~1.5 eV.
- No or less expensive and toxic elements, like In and Cd.
- Good defect properties.
- Good minority carrier life time





Photovoltaic Semiconductors

1950s
- Si

1960s
- CdTe
- GaAs

1970s
- $CuInSe_2$

1980s
- $Cu(In,Ga)Se_2$

1990s
- Cu_2ZnSnS_4

2010s
- $Cu_2ZnSn(S,Se)_4$
- $CH_3NH_3PbI_3$

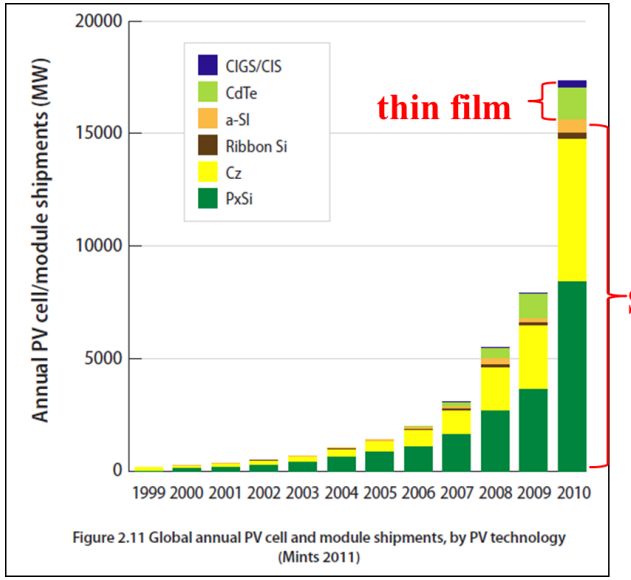
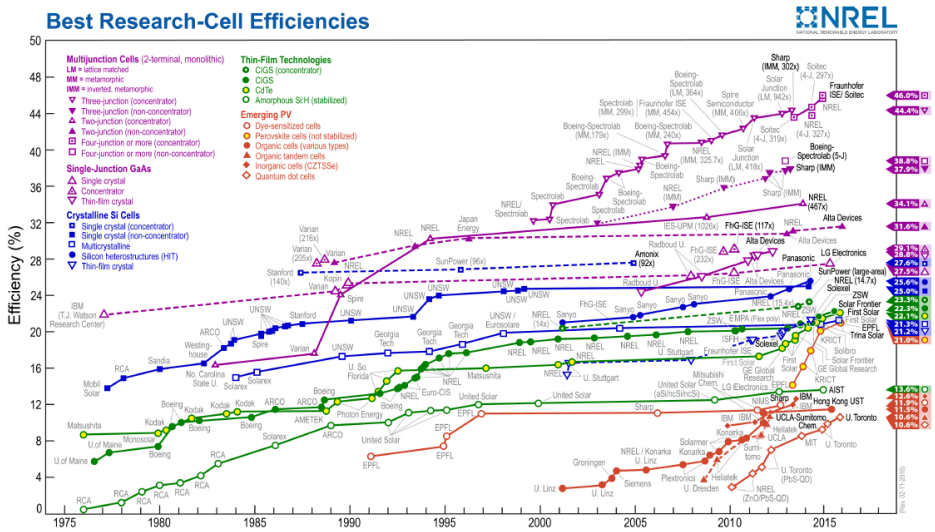
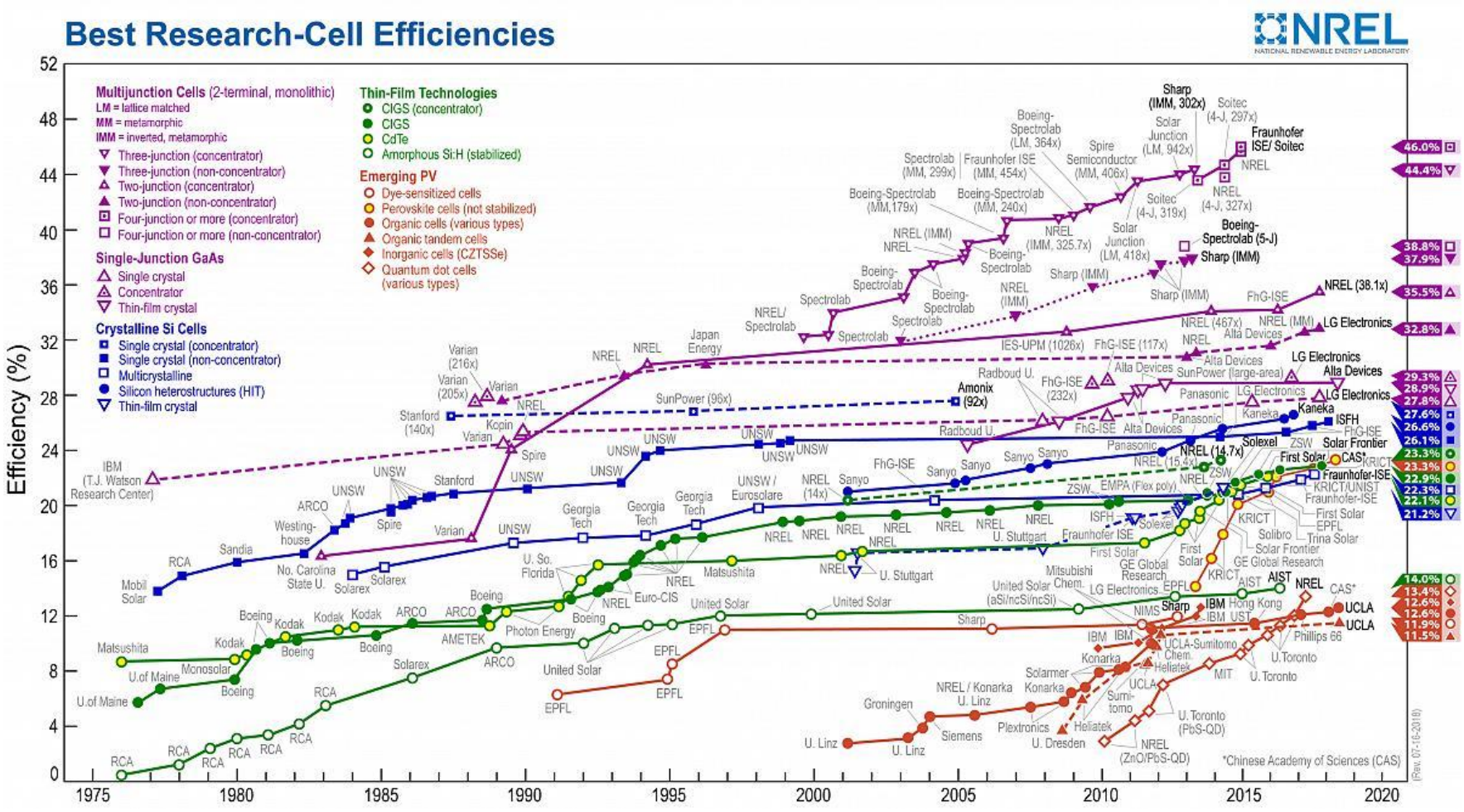


Figure 2.11 Global annual PV cell and module shipments, by PV technology (Mints 2011)

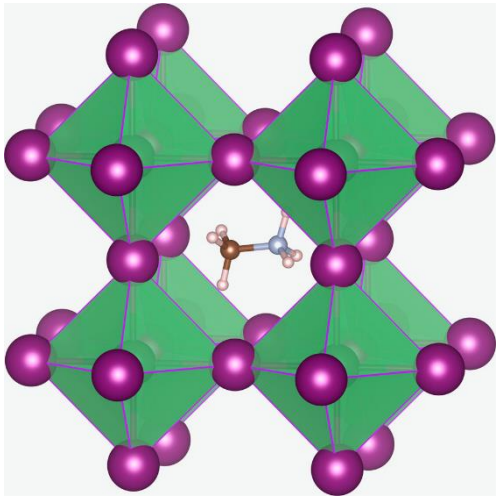


Solar Cell Efficiencies And Challenges

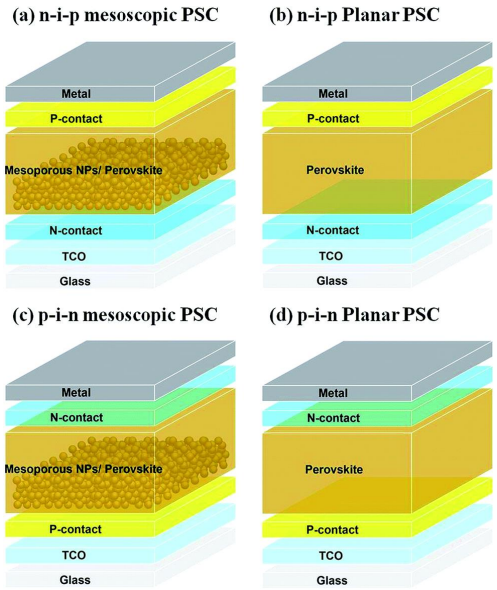


Despite great success of current solar cell technologies, due to relatively low efficiency and stability, large scale application of solar cells is still quite challenging.

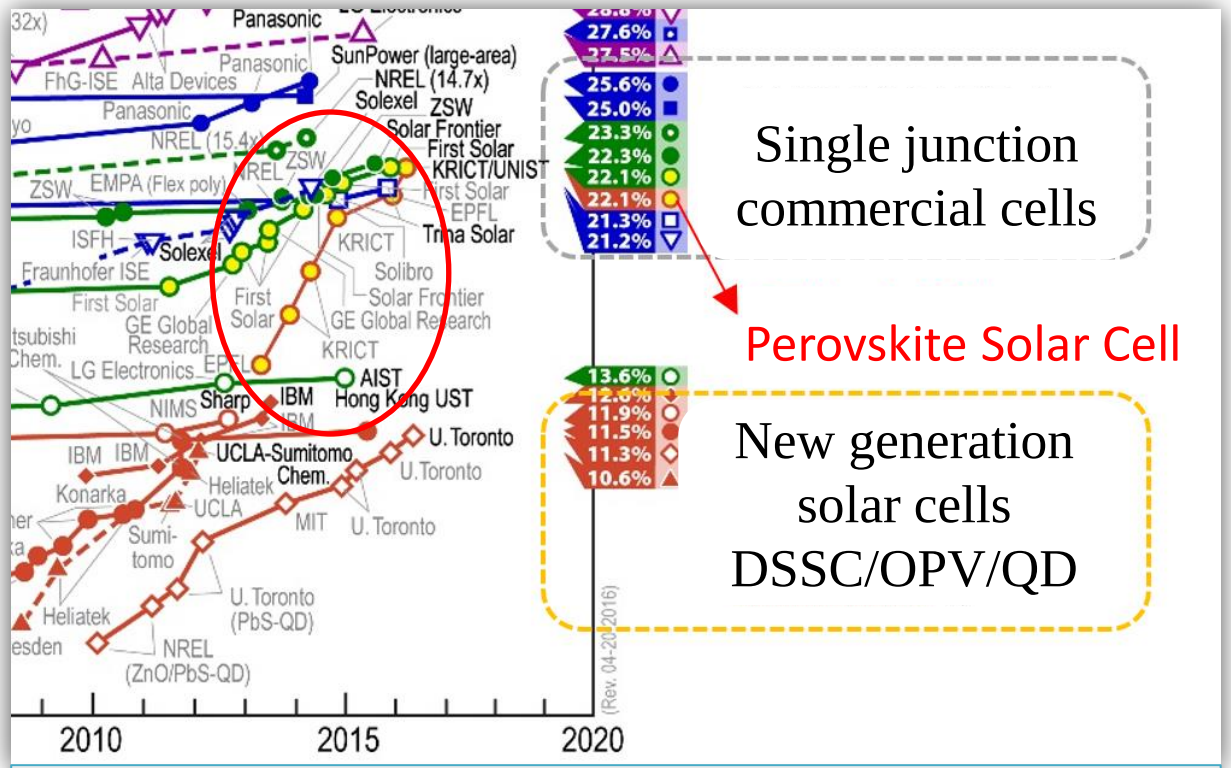
Organic-inorganic Hybrid Perovskite Solar Cell



MAPbI3



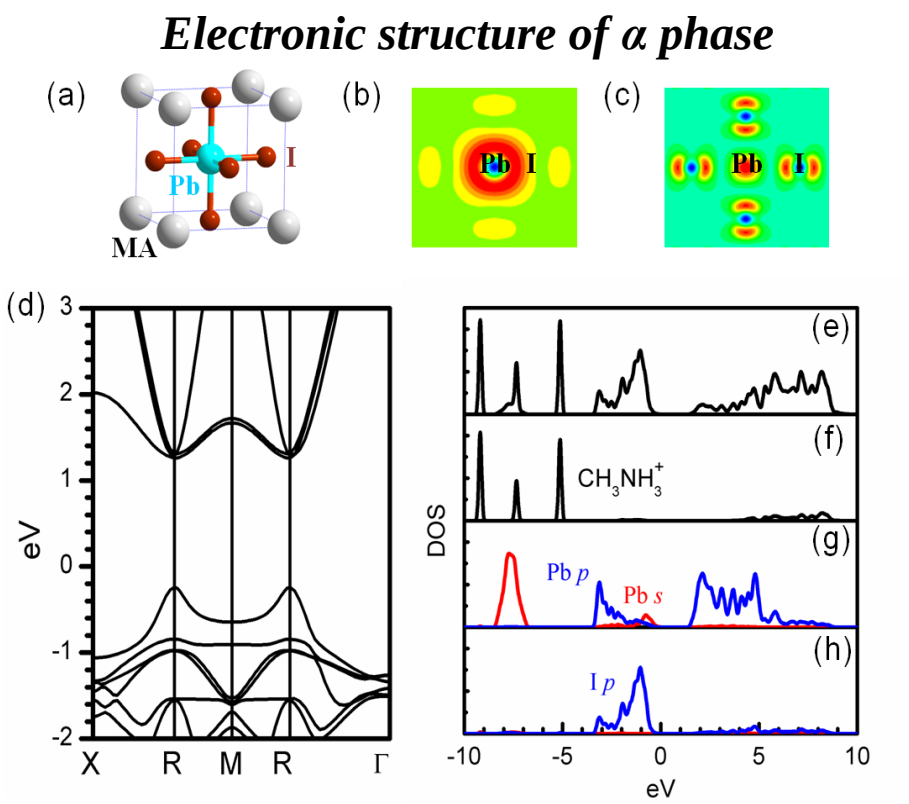
Typical Cell Structure

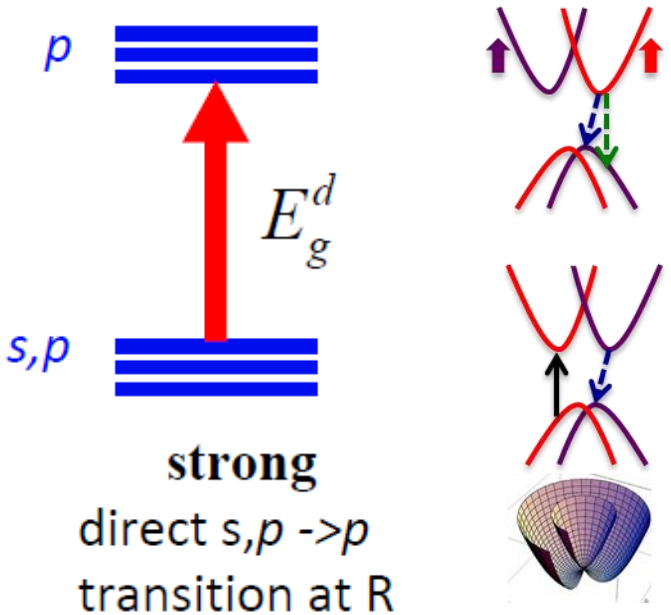


The hybrid halide perovskites have some unique optoelectronic properties, many of those are related to Pb. Its efficiency has reached over 22% in just a few years, comparable to other commercial cells.

"Halide perovskite materials for solar cells: A theoretical review", W.-J. Yin, J. Yang, J. Kang, Y. Yan, and S.-H. Wei, J. Phys. Chem. A **3**, 8926 (2015);

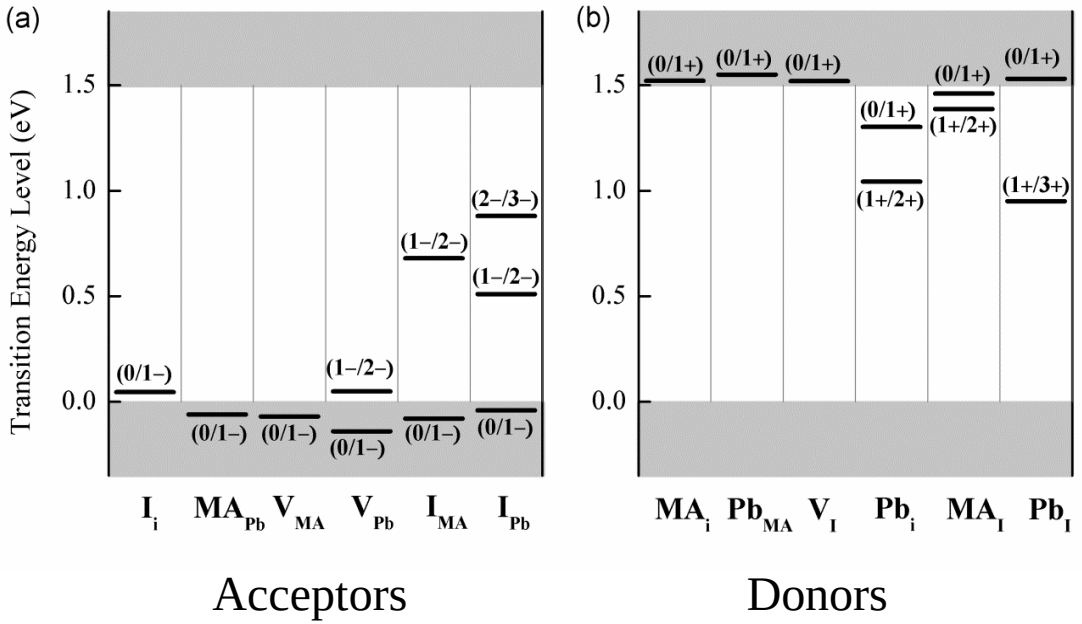
Crystal and Electronic Structures of $MAPbI_3$

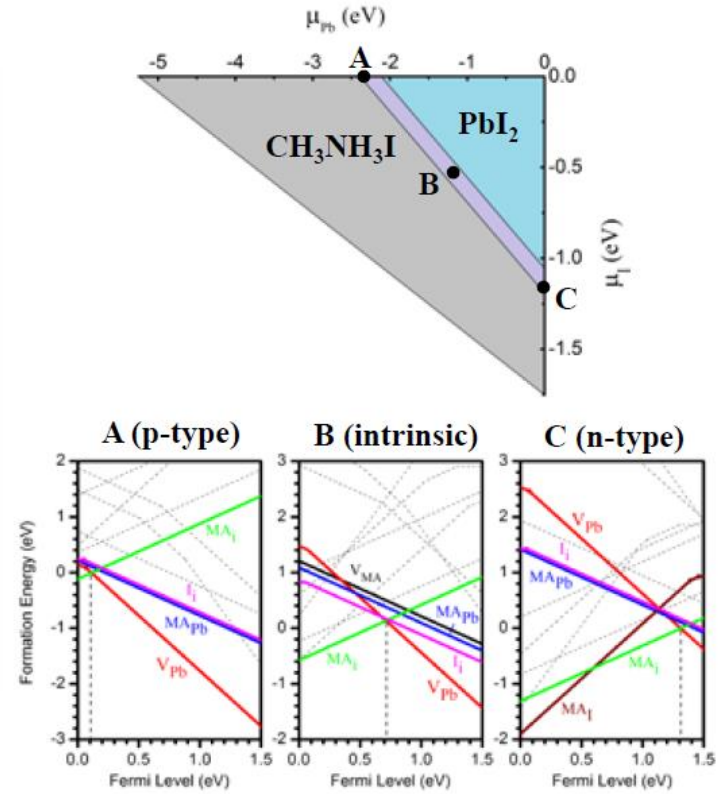




- The perovskites have inverted band structure. The VBM has anion *p*, Pb *p*+*s* characters and the CBM has non-bonding Pb *p* character.
- The high degeneracy of the band edge states and *s*,*p* wavefunction characters result in high joint DOS and large matrix elements, i.e., high absorption coefficient.
- Large SOC of Pb is also responsible for the long carrier lifetime.

Defect Formation Energy of $CH_3NH_3PbI_3$

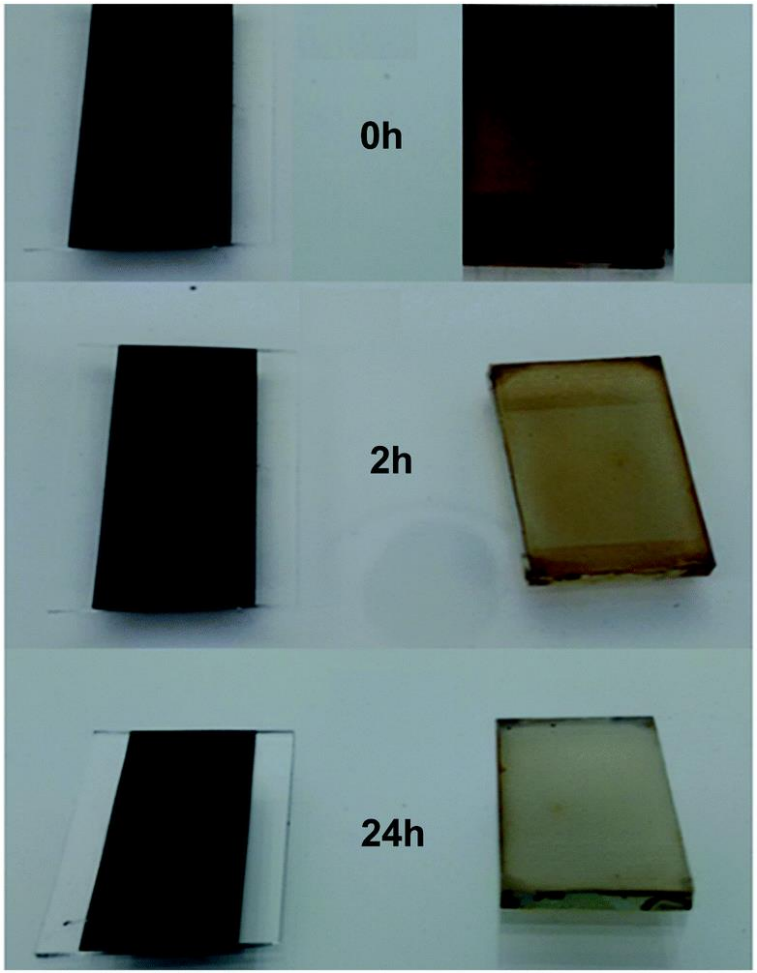




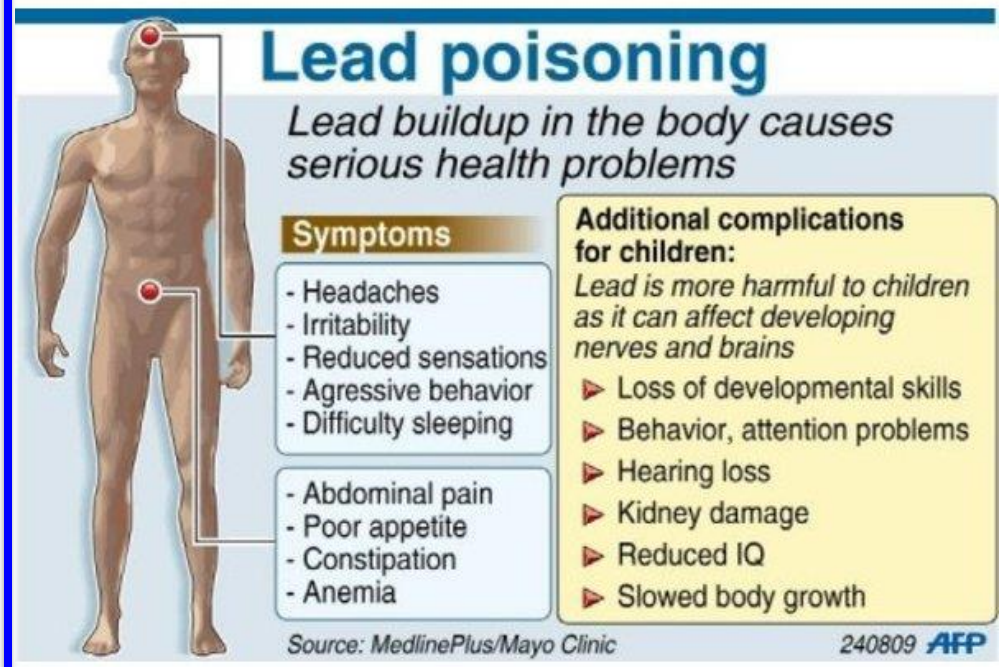
- The low energy defects have shallow defect levels whereas the defects with deep defect levels all have high formation energy. This is mainly due to the large atomic size of the elements and the ionic character of the compounds with ionization state q=1.

Main Issues Related to the Perovskites

$CH_3NH_3PbI_3 \rightarrow CH_3NH_3I + PbI_2$

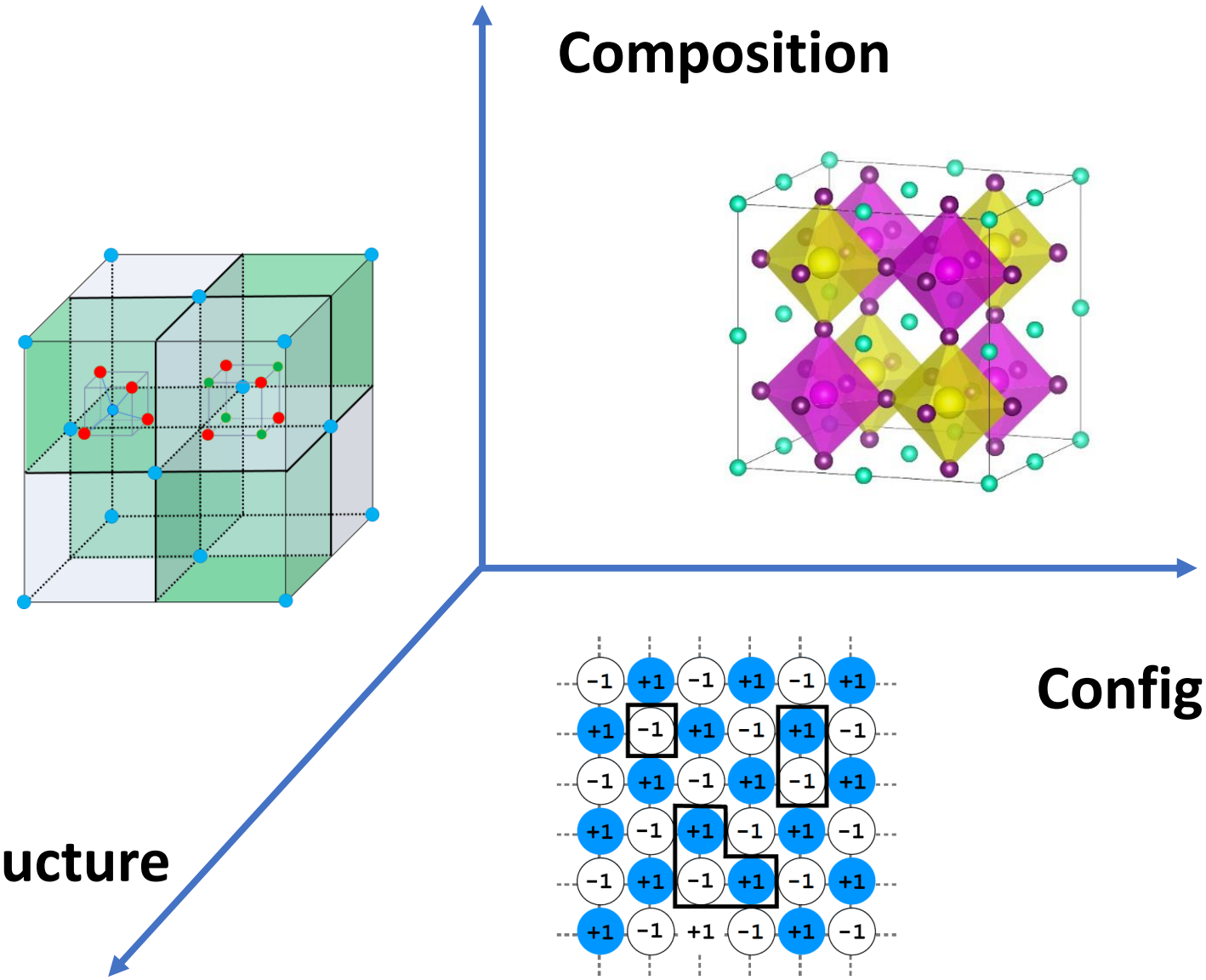


Low Stability of the Perovskites

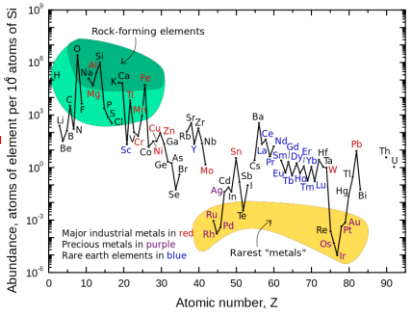


Toxicity of Pb in Solution

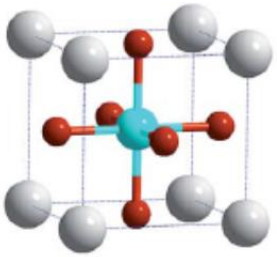
Modifying Material Properties of the Perovskites



Possible Systems That Can Be Studied:



Perovskite

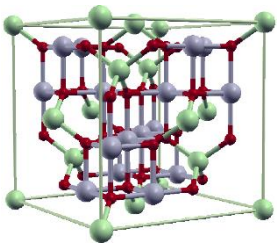


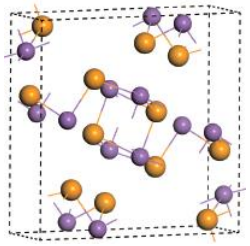
- Halides: $MAPbI_3$, $CsPbI_3$, $CsPbBr_3$
- Chalcogenides: $(Na,K,Rb,Cs)(V,Nb,Ta,Sb,Bi)(O,S,Se)_3$; $(Mg,Ca,Sr,Ba)(Ti,Zr,Hf,Si,Ge,Sn)(O,S,Se)_3$
- Pnictogenides: $(Ti,Zr,Hf,Si,Ge,Sn)(V,Nb,Ta,Sb,Bi)(N,P,As)_3$; $(Sc,Al,Ga,In)(Cr,Mo,W)(N,P,As)_3$
- Isovalent Alloys: $(MA,FA,Cs)(Pb,Sn,Ge)(I,Br,Cl,F)_3$
- Atomic Transmutation: $(Na,K,Rb,Cs)_2(CuAg,Au)(Sb,Bi,Sc,Y)(I,Br,Cl)_6$; $(Na,K,Rb,Cs)(Sb,Bi,Sc,Y)(O,S,Se)(I,Br,Cl)_2$; $(Mg,Ca,Sr,Ba)_2(Sc,Al,Ga,In)(V,Nb,Ta,Sb,Bi)\ (O,S,Se)_3$

Other Systems

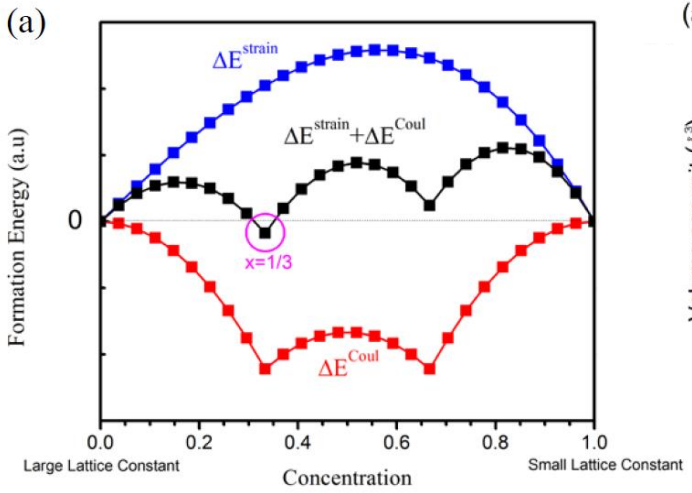
AB_2X_4 Spinels, Heusler

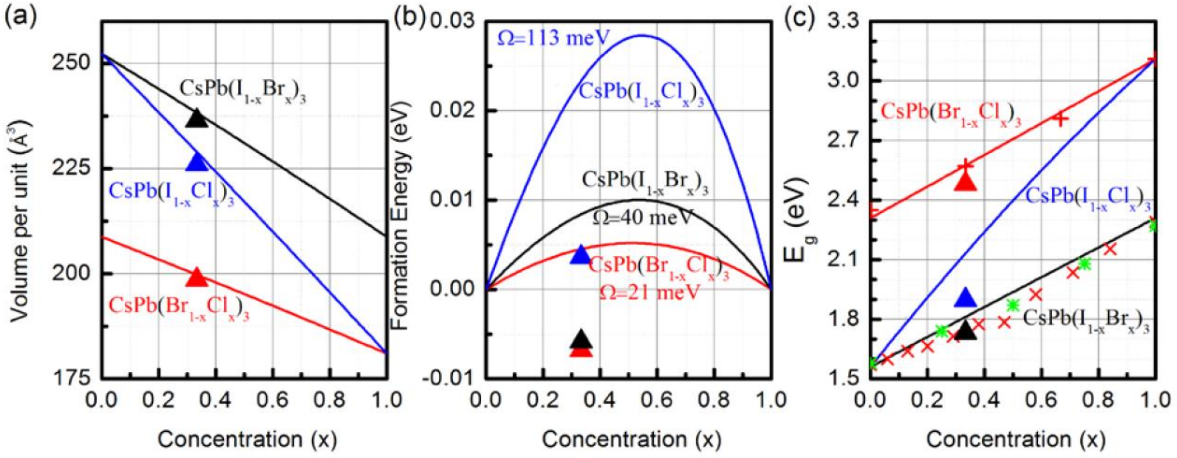
$(Cu,Ag)_x(Sb,Bi)_y(S,Se)_z$

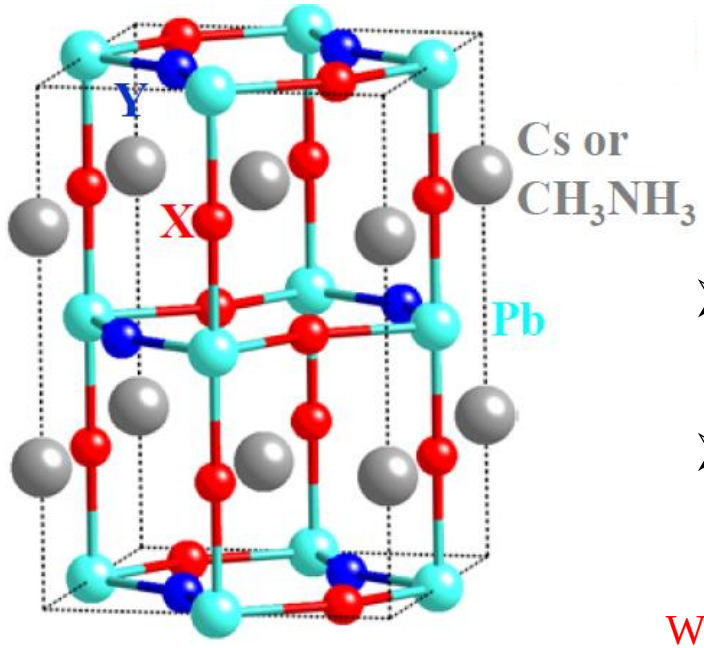




Stabilize Perovskite Structure by Alloying Anions



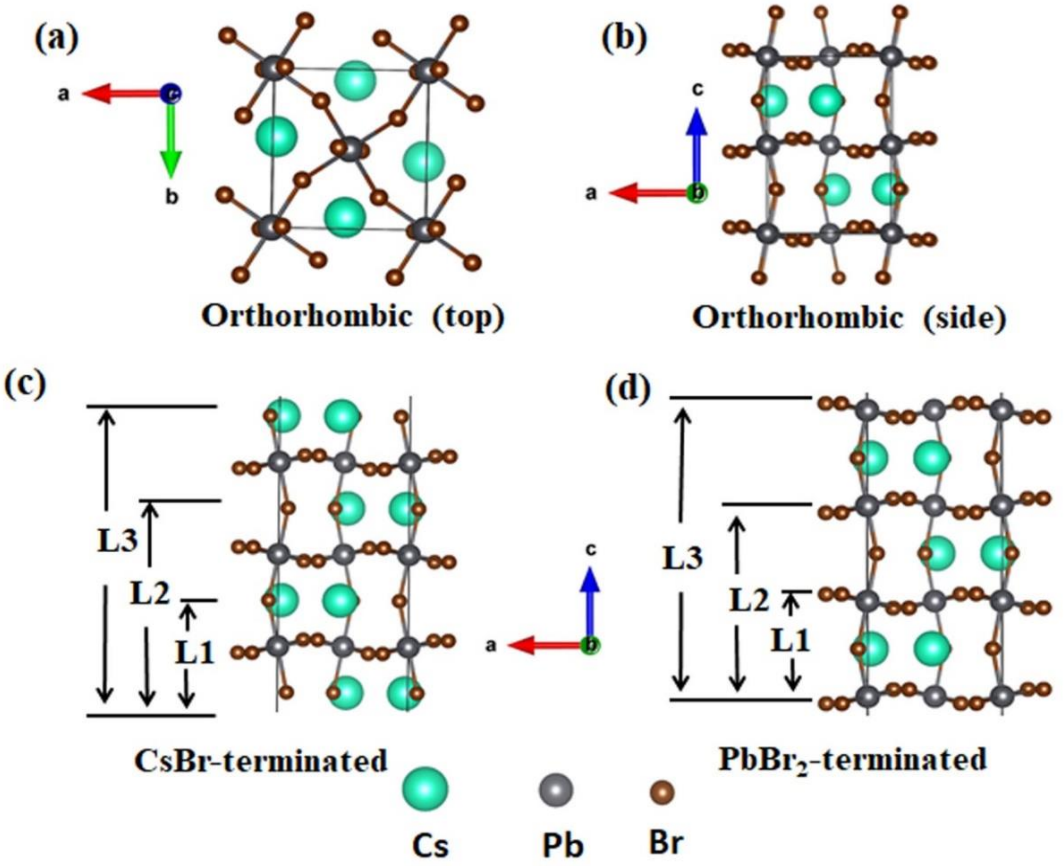


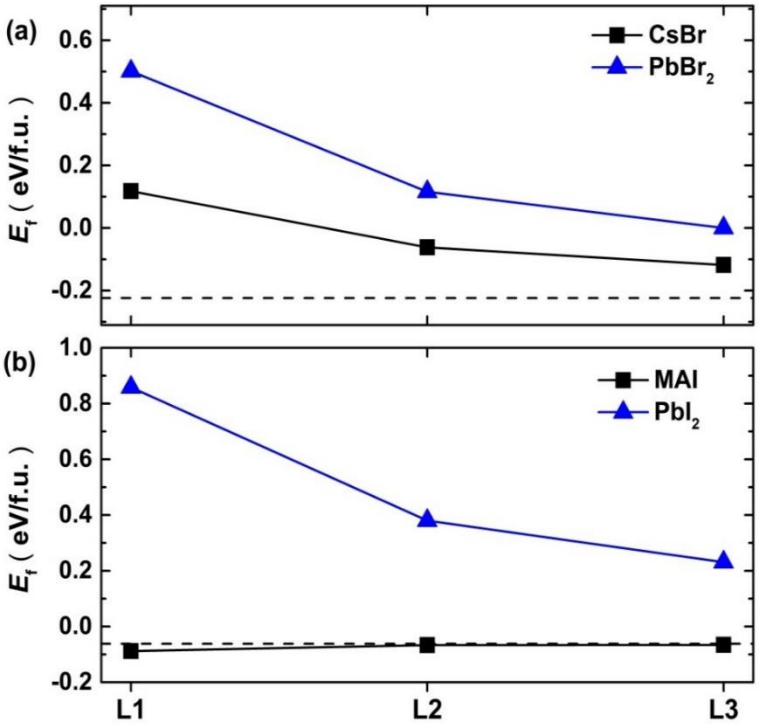


- The variations of formation energies and band gaps of the mixed random halide alloys $CsPbX_{1-x}Y_x$ show unusual behaviors such as small or even negative formation energies at some concentrations and negligible or even negative band gap bowing.
- Formation of mixed-(I, Cl) alloy is difficult but forming mixed-(Br, Cl) and (I, Br) alloys are easy.
- The very stable ordered structures at x=1/3 is due to combined effects of strain and Coulomb interactions.

W.-J. Yin, Y. Yan, and S.-H. Wei, J. Phys. Chem. Lett. 5, 3625 (2014).

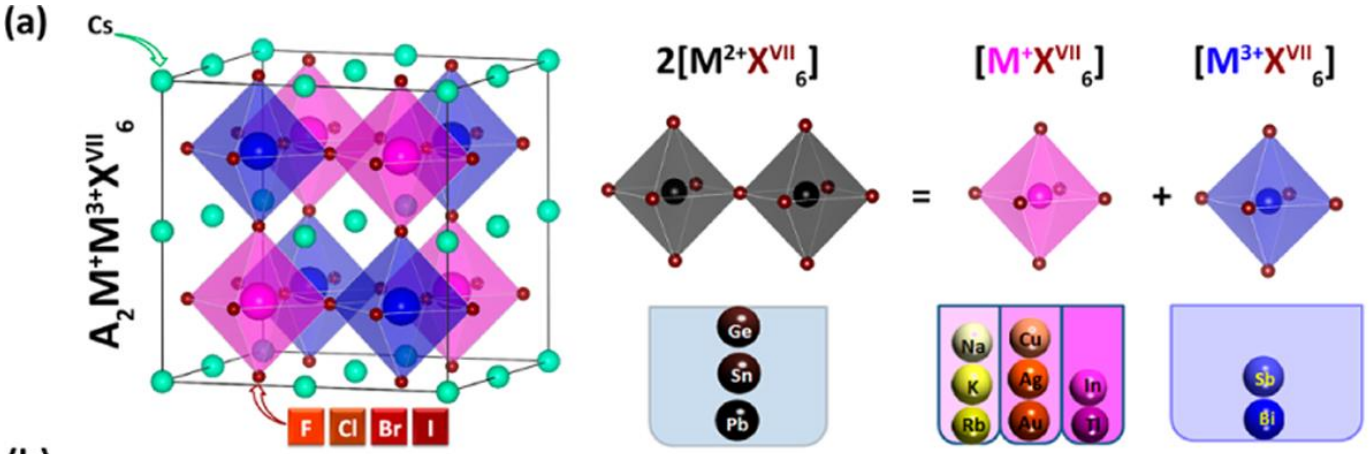
Improve the Stability of Perovskite by Extracting a 2D Slab from the 3D Perovskites





Cleaved structure within (001) plane leads to two termination: CsBr- and $PbBr_2$. One of the surface could have low energy.

Atomic Transmutation Derived Double Perovskite



(b)

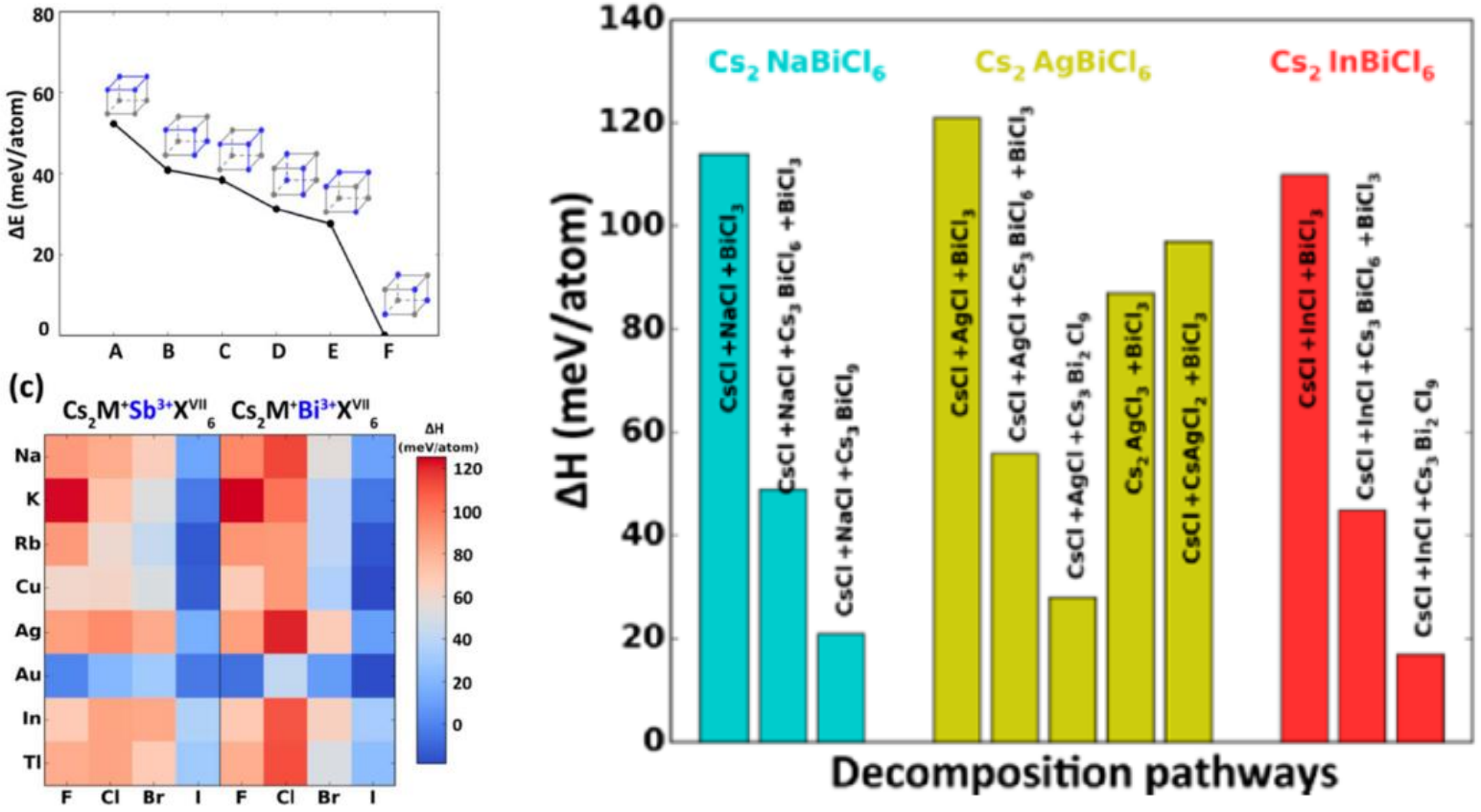
	Group IA			Group IB			Group IIIA	
M^+	Na^+	K^+	Rb^+	Cu^+	Ag^+	Au^+	In^+	Tl^+
ΔH (>0 meV/atom)								
Band Gap (0.8~2.0 eV)								
m_e^*, m_h^* ($\|m\| < 1.0\ m_e$)								
ΔE_b (<100 meV)								
Promising Compounds				✓ ✓ ✓	✓ ✓ ✓	✓ ✓ ✓	✓ ✓	

	F	Cl	Br	I
Sb				
Bi				

✓ Optimal
Selected
Abandoned

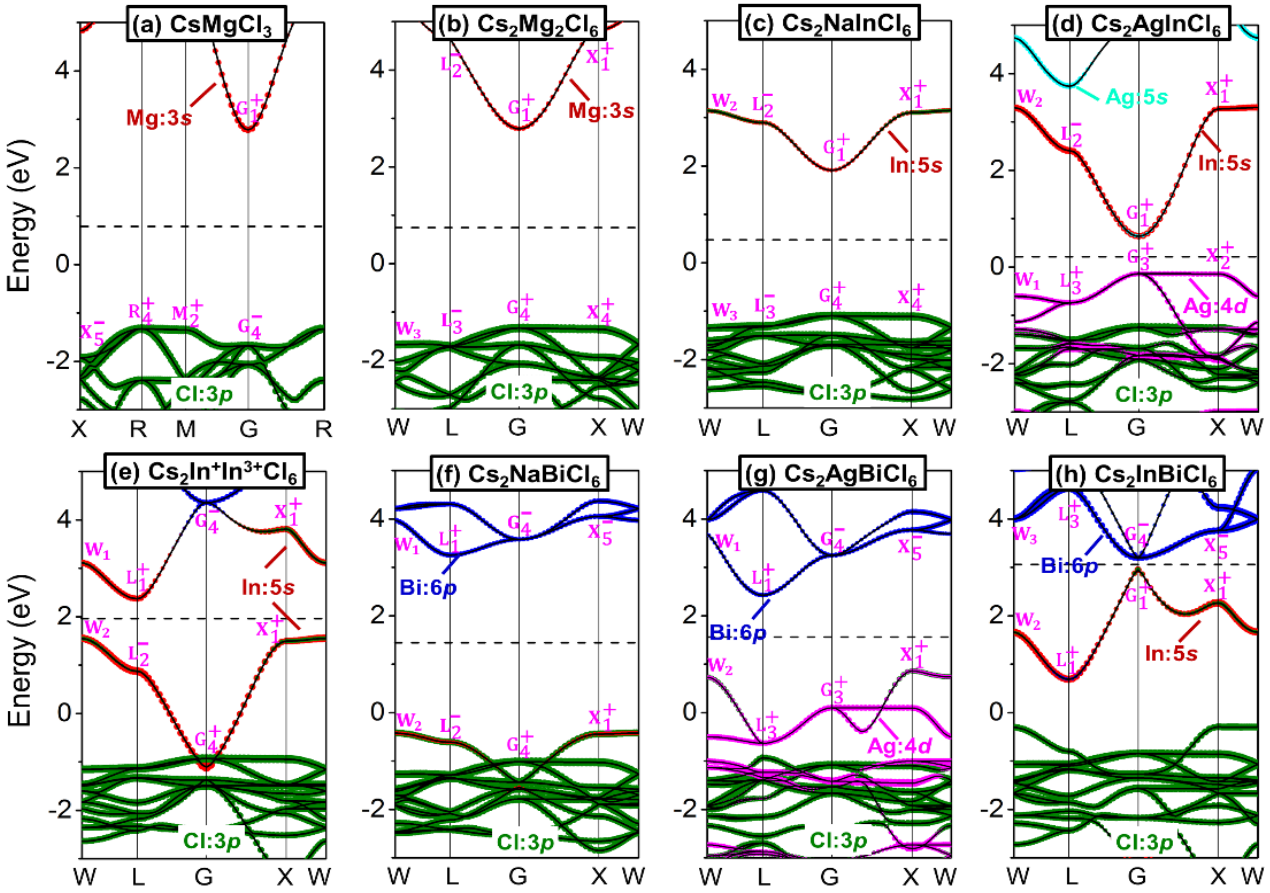
X. Zhao, et al. J. Am. Chem. Soc. **139**, 2630 (2017).

Decomposition Entropy Associated with Decomposition Pathway



- Many compounds in double perovskite structure are stable against decomposition into binary and ternary compounds.

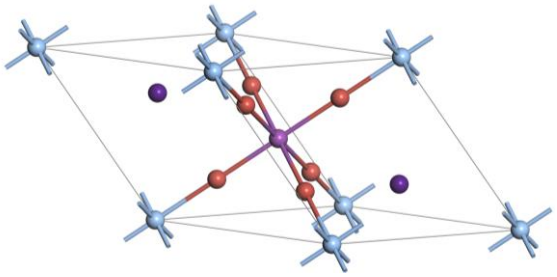
Symmetry Properties of the Band Structures of Ordered Double Perovskite Compounds

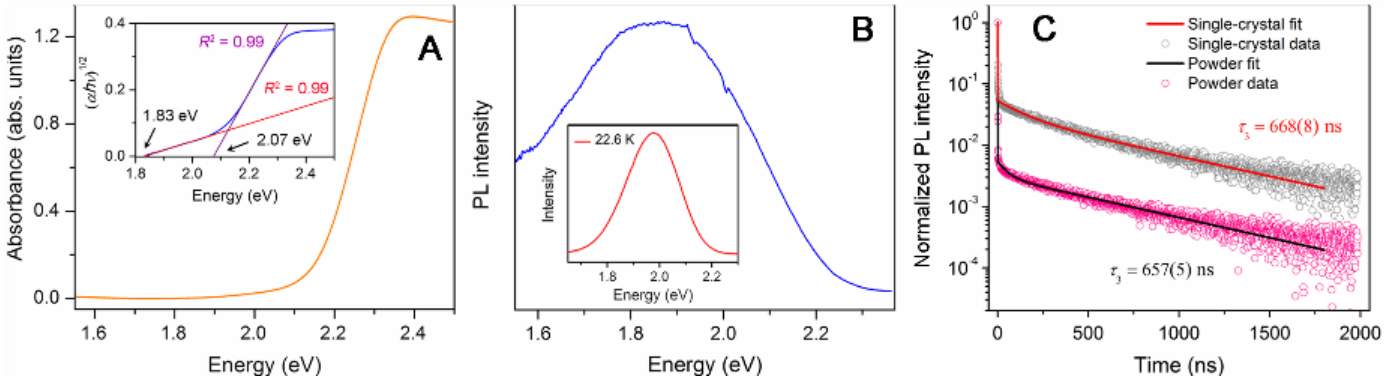


- To obtain superior optoelectronic properties, both of the B^{+}/B^{3+} cations in $A_2B^{+}B^{3+}X_6$ must possess the lone-pair *s* states, so that a strong *s*-*p* coupling between the lone-pair *s* and X *p* orbitals could occur.

P. Zhang, J. Yang, and S.-H. Wei*, J. Mater. Chem. A. **6**, 1809 (2018).

Indirect Band Gap of Ordered $Cs_2AgBiBr_6$

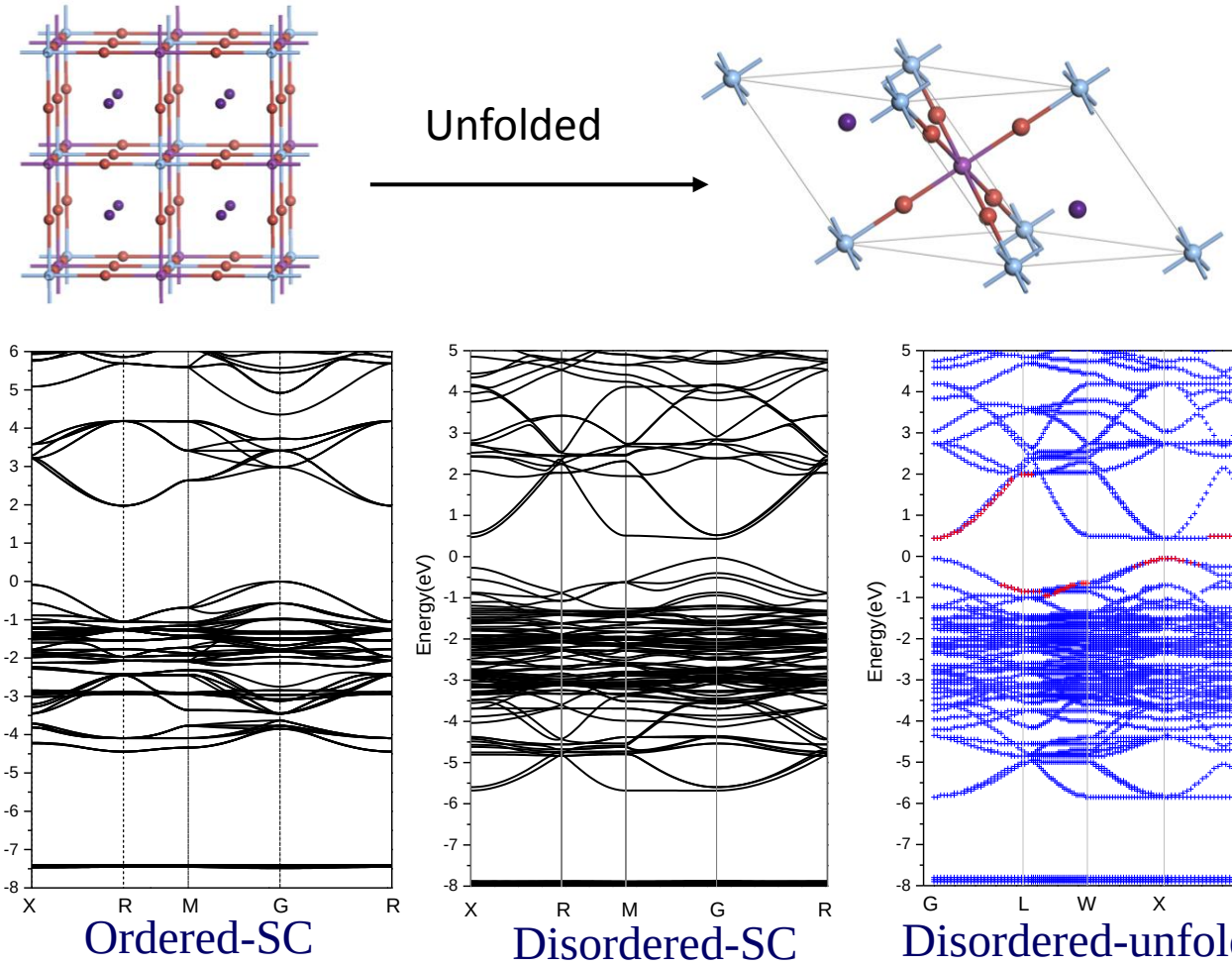




- Recently, $Cs_2AgBiBr_6$ has been found to be stable and characterized as indirect band gap of 1.95 eV by photoluminescence spectroscopy.

A. Slavney et al., J. Am. Chem. Soc. **138**, 2138 (2016).

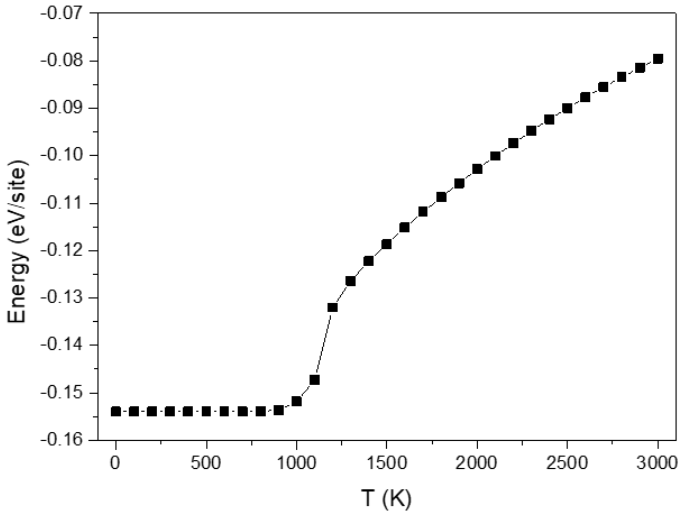
Ordering Effects on the Band Structure of $Cs_2AgBiBr_6$

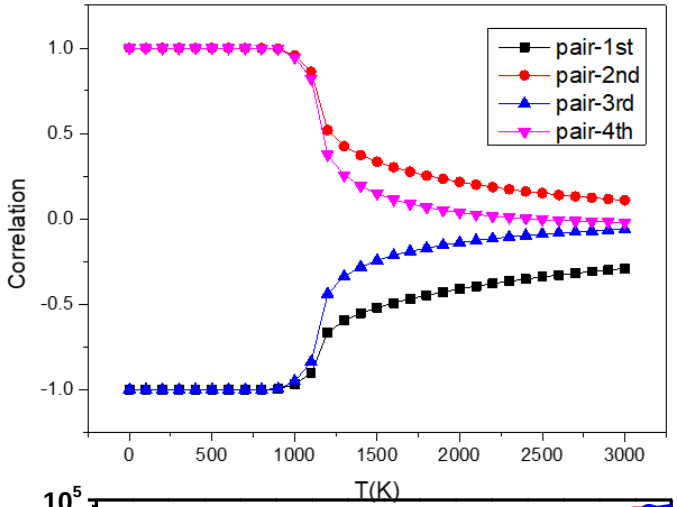


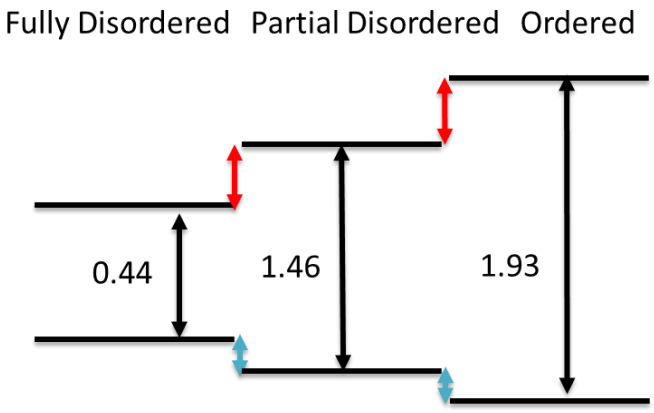
- Reduced symmetry in disordered structure can significantly lower the band gap and convert an indirect semiconductor to direct (pseudodirect) semiconductor.

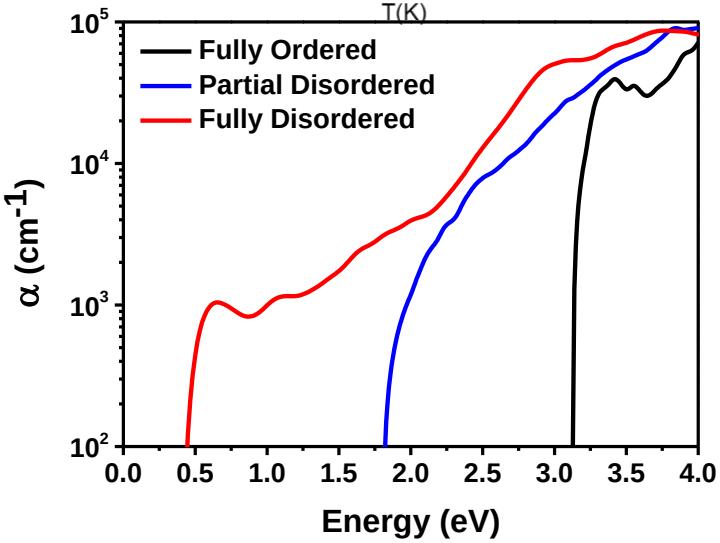
J. Yang, P. Zhang, and S.-H. Wei, J. Phys. Chem. Lett. 9, 31 (2018).

Control the Band Gap and Optical Transitions of $Cs_2AgBiBr_6$ by Controlling the Ordering Parameters



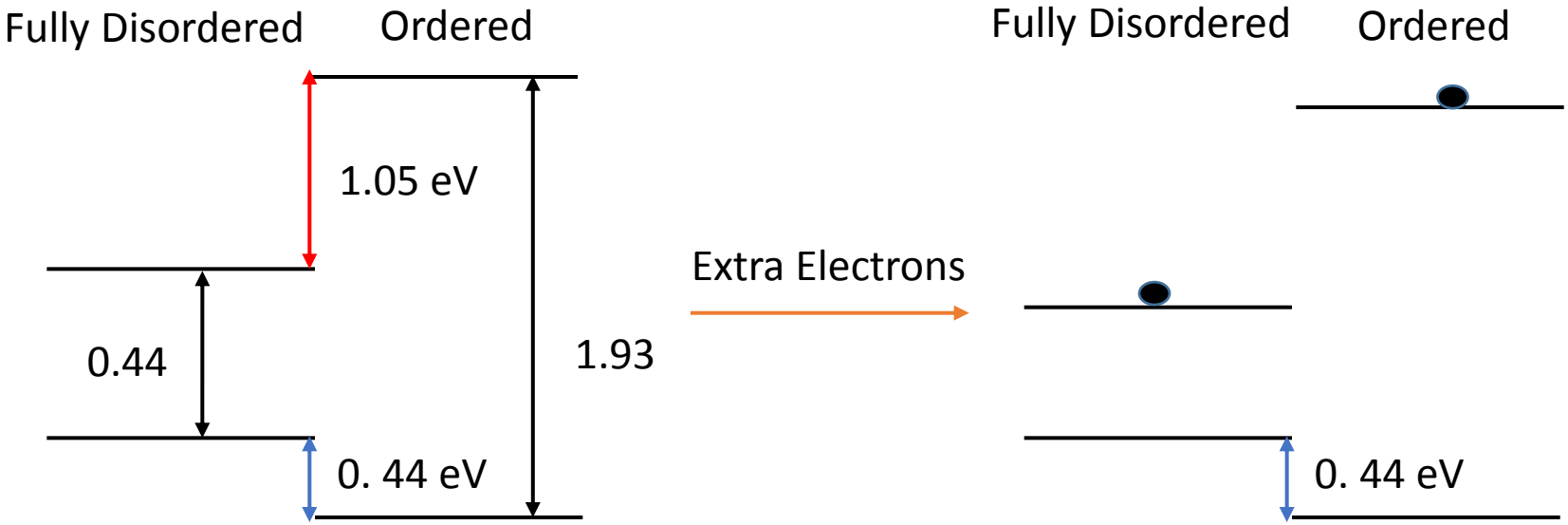






- Bandgap and optical transitions are function of ordering parameter, which can be controlled by growth temperature.

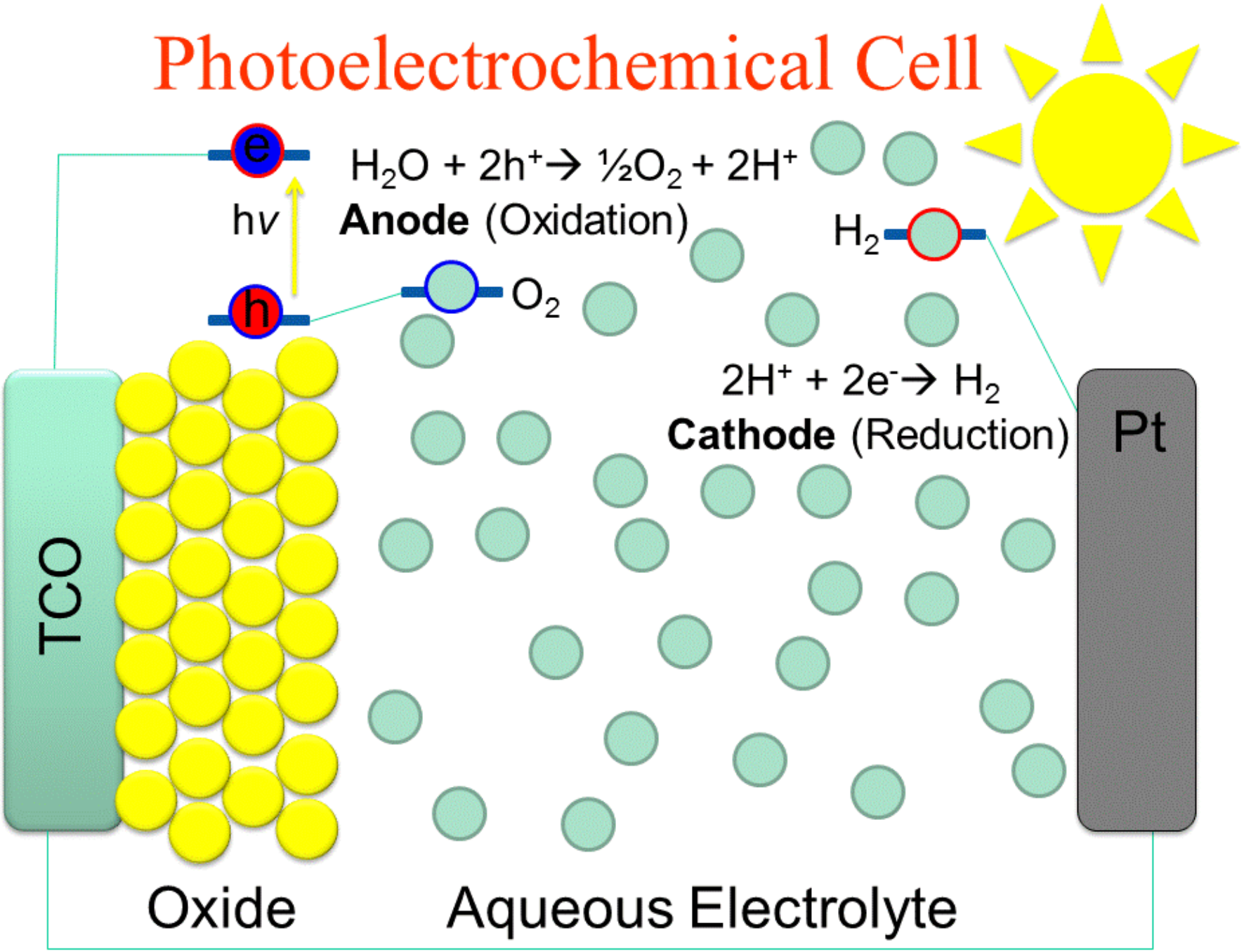
Control the Band Gap and Optical Transitions of $Cs_2AgBiBr_6$ by Controlling the Ordering Parameters



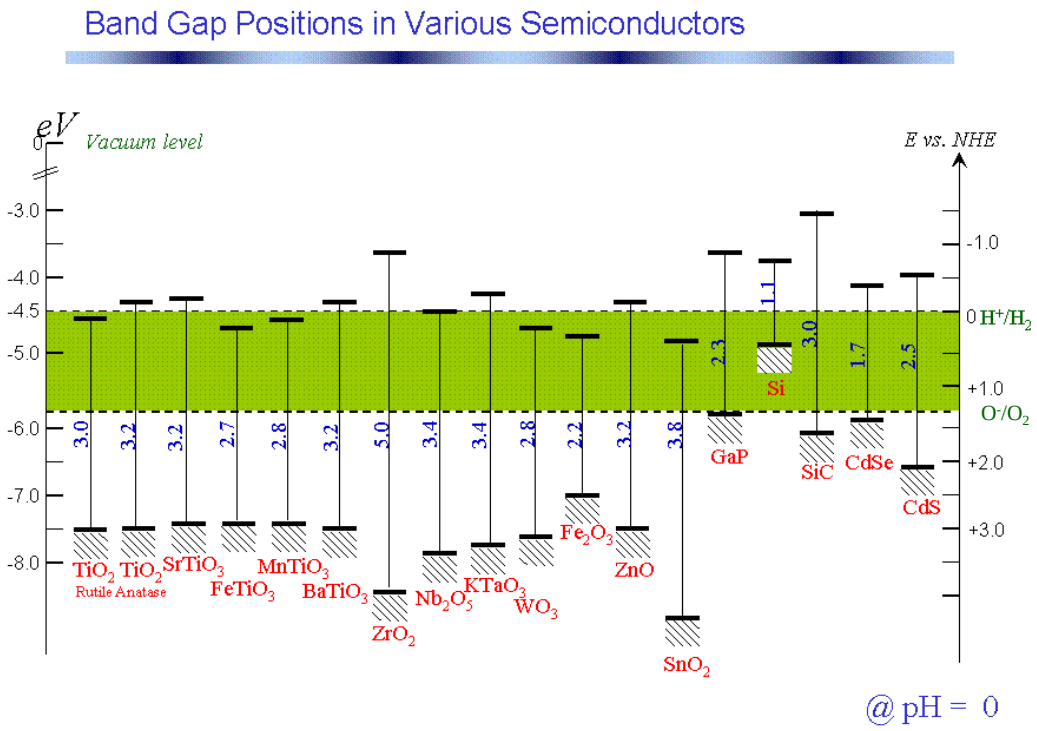
- Doping such as Ba_{Cs}, La_{Cs} or creating Cs vacancy etc. could reduce the energy difference between ordered and disordered structure or even make disordered structure more stable than ordered structure, reduce transition temperatures.

J. Yang, P. Zhang, and S.-H. Wei, J. Phys. Chem. Lett. 9, 31 (2018).

Design Oxides for Hydrogen Production through PEC Water Splitting

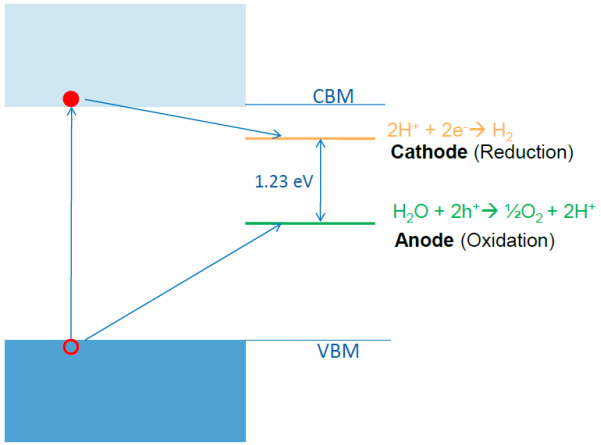

Photoelectrochemical Cell
e
hν
h
$H_2O + 2h^+ \rightarrow ½O_2 + 2H^+$
Anode (Oxidation)
O_2
H_2
$2H^+ + 2e^- \rightarrow H_2$
Cathode (Reduction)
TCO
Pt
Oxide
Aqueous Electrolyte

Material Choices for PEC Water Splitting



PEC catalyst criteria

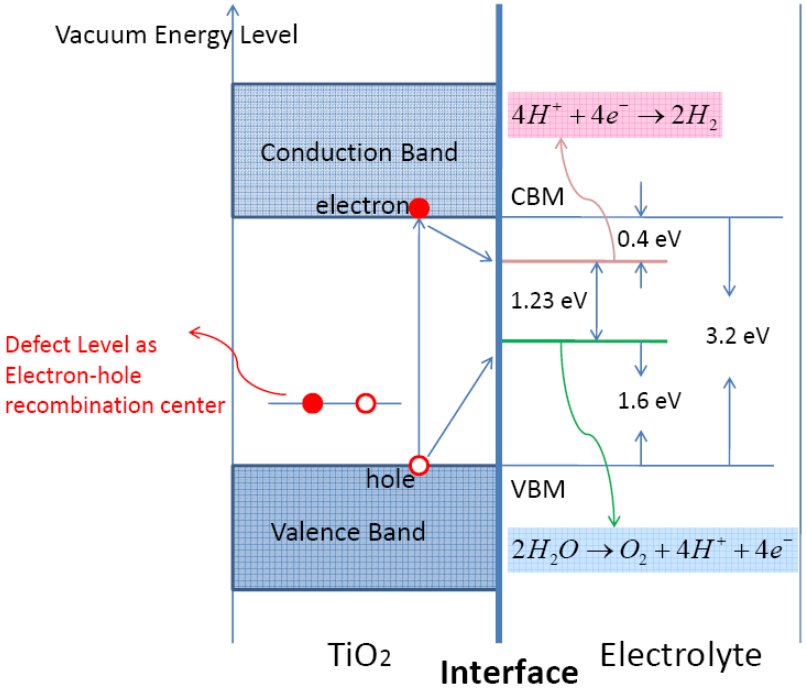
- Structural **stability** in solution.
- High **availability** (low cost).
- Good **catalytic** activity.
- **Band gap**: 1.7 – 2.2 eV.
- High **Photocurrent** generation.
- Band-edge **alignment**.

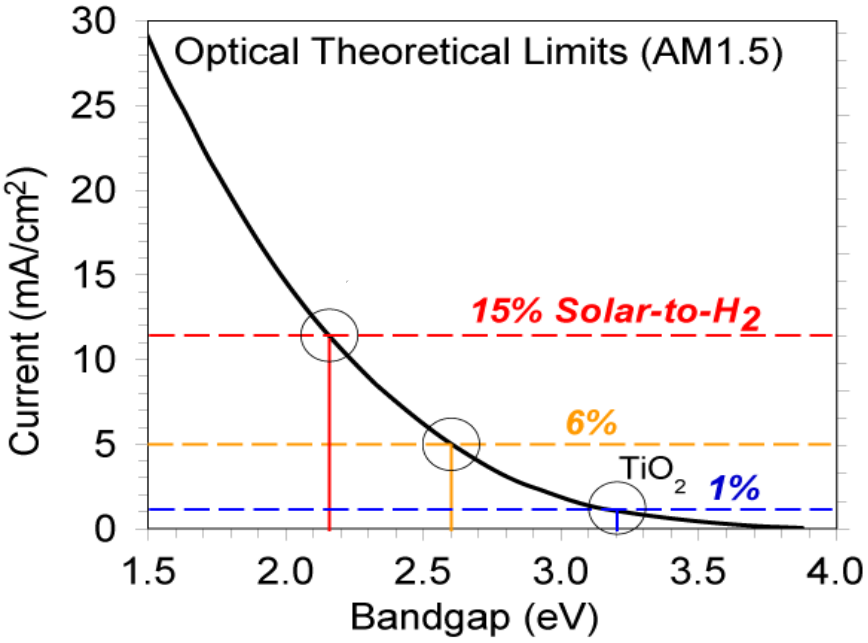


None of the common compounds meet the criterions.

Band structure engineering is needed.

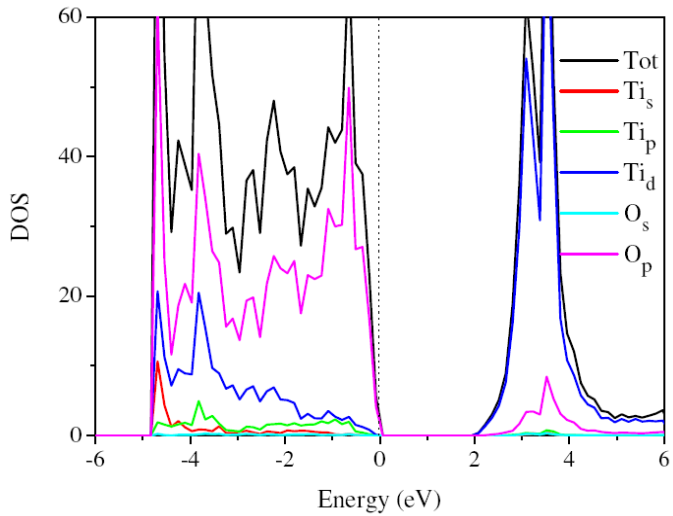
Anatase TiO_2 for PEC Water Splitting



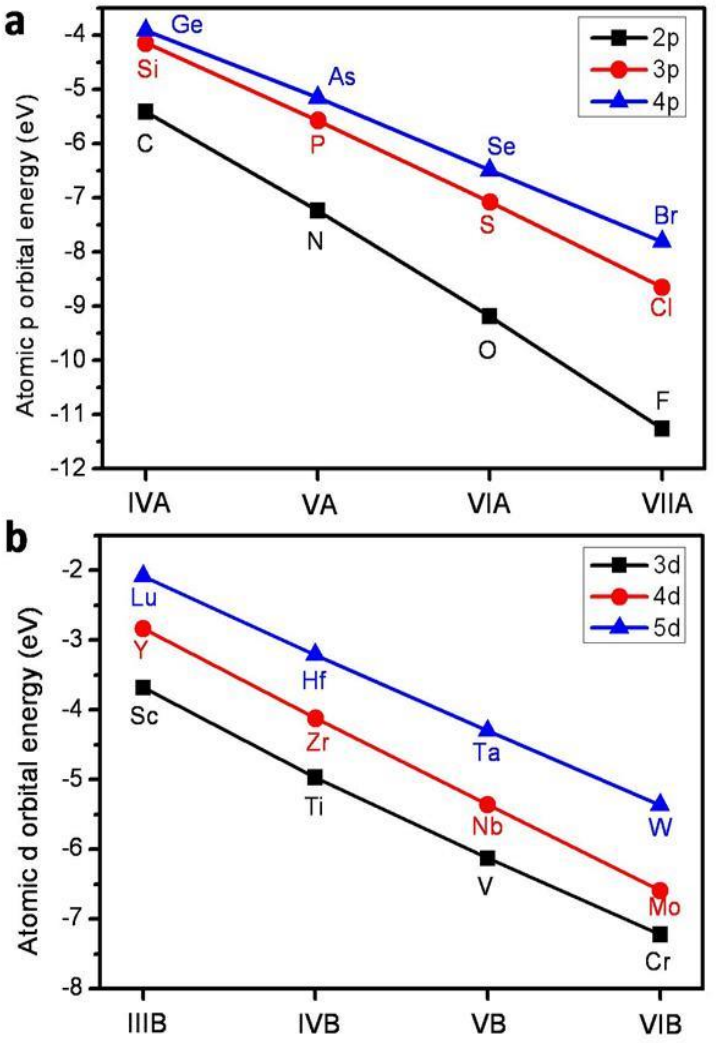


- TiO_2 is one of the most studied oxides for water splitting. It satisfy most of the criteria except that its band gap is too large to absorber visible light so the generated photocurrent is low.

Rational Band Structure Engineering



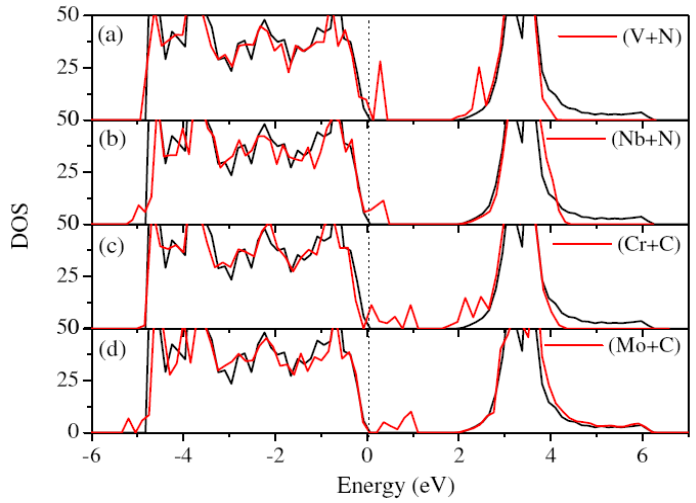
Chemical trend of atomic orbital energy

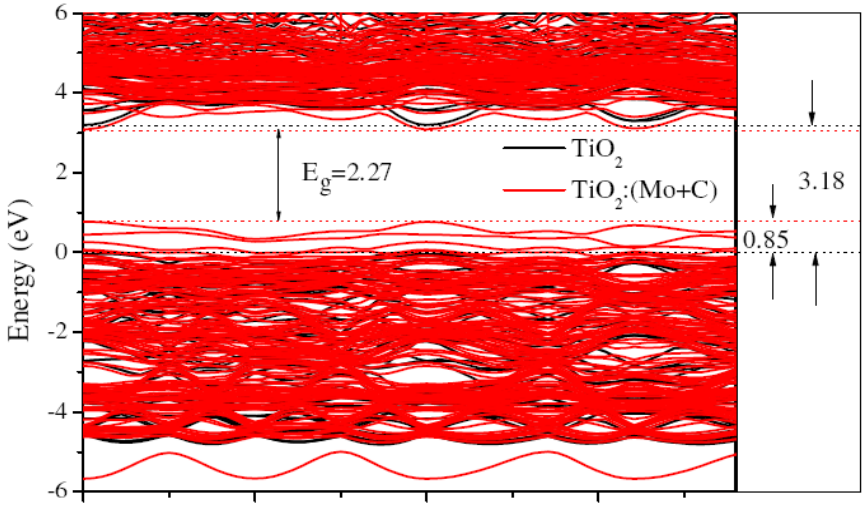


Identify atomic wavefunction characters of the band edge states

- VBM has anion O, *p* character
- CBM has cation Ti, d character
- The defect bands should raise the VBM but not reduce the CBM
- Charge compensated defect pairs should be used to reduce carrier recombination.

TiO_2:(C+Mo) for PEC Water Splitting





[Y Gai et al., Phys. Rev. Lett. **102**, 036402 (2009)]

Mo + C Codoped TiO_2 Using Thermal Oxidation for Enhancing Photocatalytic Activity

VOL. 2 • NO. 4 • 1173–1176 • 2010

ACS APPLIED MATERIALS & INTERFACES

1173

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Key Laboratory of Artificial Micro- and Nano-structures of Ministry of Education and School of Physics and Technology and Center for Electron Microscopy, Wuhan University, Wuhan 430072, P.R. China

ABSTRACT The photocatalytic activity of TiO_2 is enhanced mainly through heightening absorption of UV−vis light and improving the separation efficiency of photoinduced electrons and holes. The recent new theoretical research revealed that the TiO_2 codoped with Mo + C is considered to be an optimal doping system. On the basis of this theory, the Mo + C codoped TiO_2 powders were first experimentally synthesized by thermal oxidizing a mixture of TiC and MoO_3 powders in the air. The XRD patterns and the XPS survey spectrum showed that carbon (C) acted as a Ti−O−C band structure and molybdenum (Mo) existed as Mo^{6+} in anatase TiO_2. The Mo+C codoped TiO_2 had a 32 nm red shift of the spectrum onset compared with pure anatase TiO_2, and its band gap was reduced from 3.20 to 2.97 eV. The photocurrent of the Mo + C codoped TiO_2 was about 4 times as high as that of pure anatase TiO_2, and its photocatalytic activity on decomposition of methylene blue was enhanced.

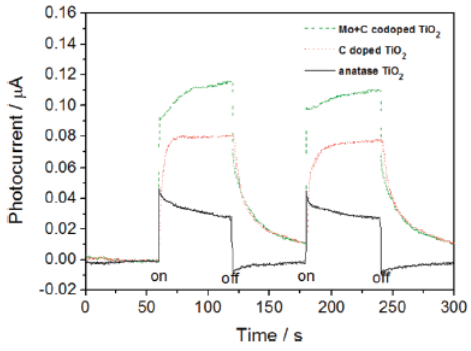
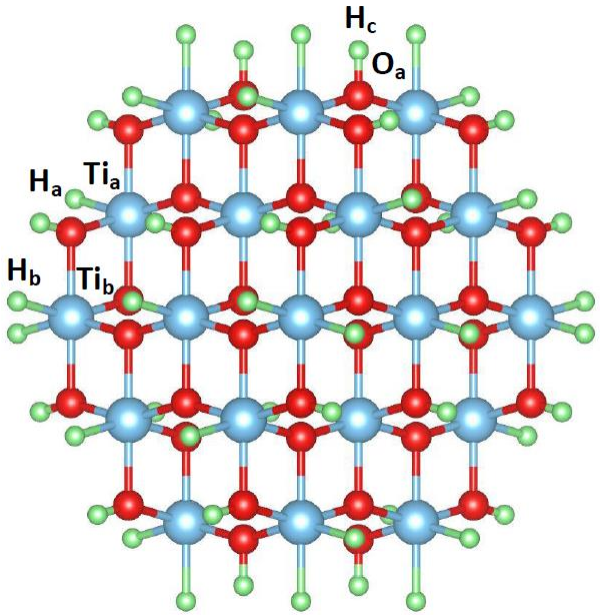


FIGURE 4. Photoelectrochemical responses of Mo + C codoped TiO_2, C-doped TiO_2, and anatase TiO_2.

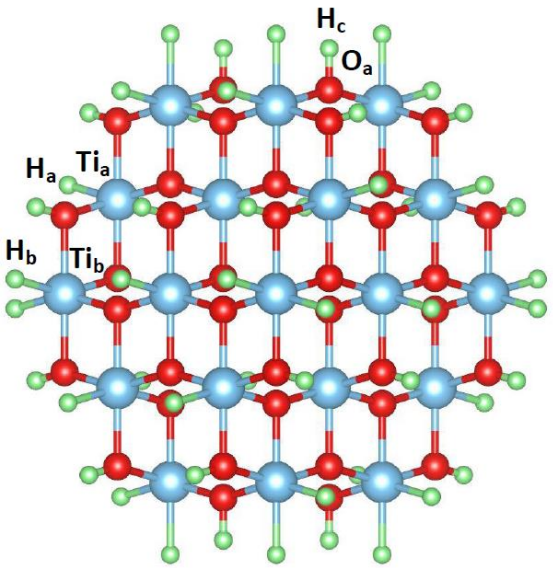
Reduce the Band Gap of Nano Metal Oxides



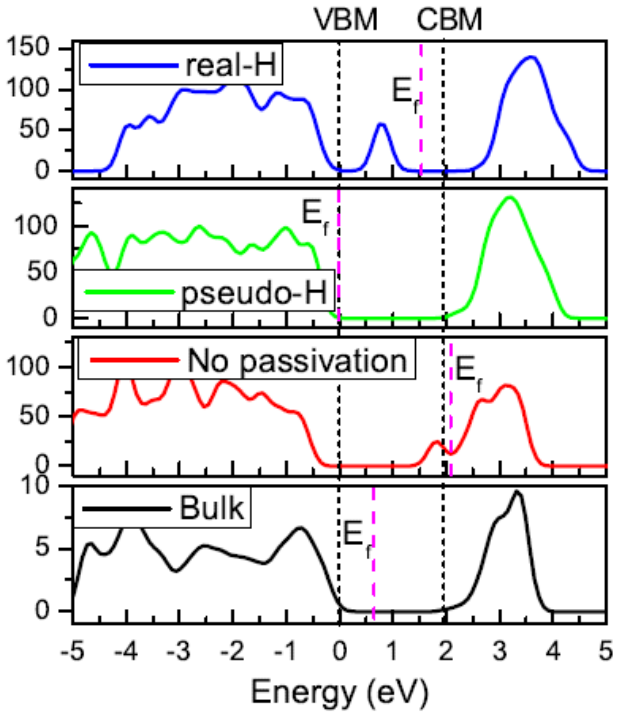
- Nano materials have large surface/bulk ratio, therefore, is more suitable for catalytic applications

- Most of the oxides have too large band gap for a specific application. Can the band gap of a nano structured material be reduced comparing to its bulk form?

Passivated Anatase TiO_2 QD



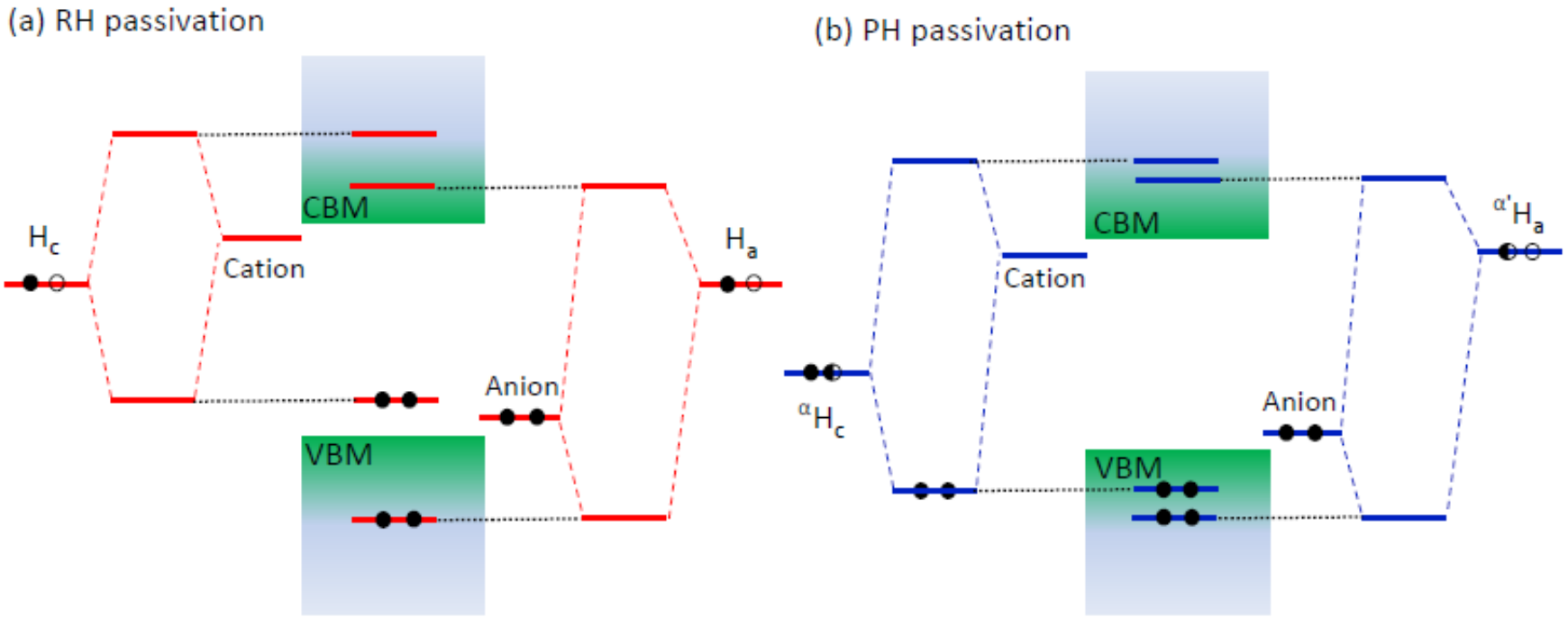
Total DOS



Pseudo-H passivation removes the mid-gap state and increase the band gap due to quantum confinement effect.

Real-H atoms cannot provide enough electrons to saturate each Ti dangling bonds, therefore, it can produces defect levels derived from H and Ti orbitals inside the gap .

Real H Passivation vs. Pseudo H Passivation on the Electronic Structure of Ionic Semiconductors



It is possible to reduce the band gap of a low dimensional oxides with real hydrogen passivation!

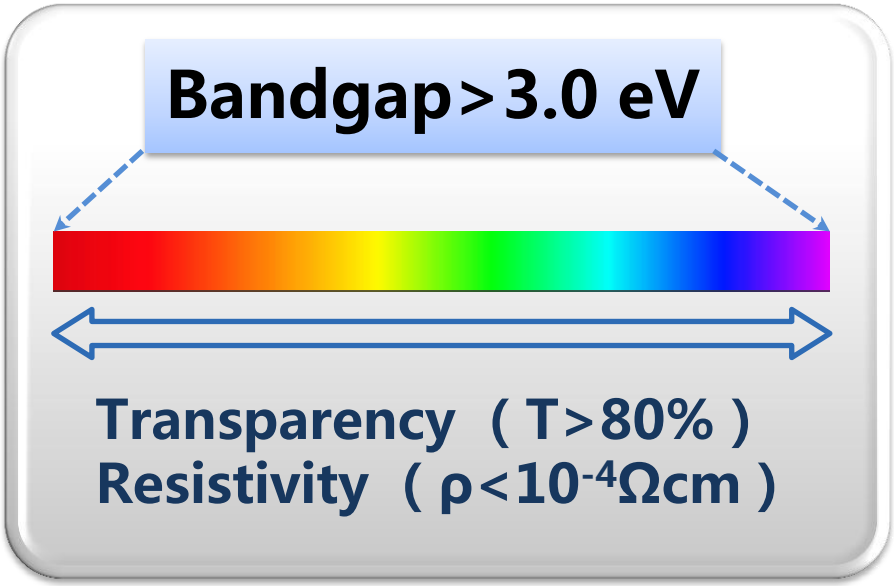
H.-X. Deng, S.-S. Li, J. Li, S.-H. Wei, Phys. Rev. B **85**, 195328

Design Bipolar Dopable Transparent Conducting Oxides

Transparent Conducting Materials

TCMs

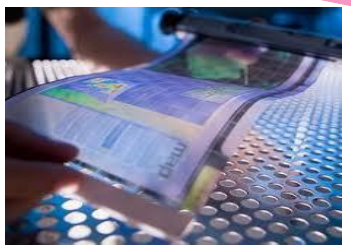
- **High conductivity**
- **High visible light transparency**



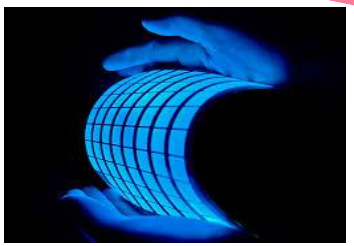
Applications of the TCMs

Display Pannel

Smart window



Flexible transparent device



Organic LEDs

Solar cells

Development of TCOs

1900 … 1950 1960 1970 1980 1990 2000 2010 2016

CdO

SnO_2,SnO_2:Cl,SnO_2:Sb

In_2O_3:Sn

CdSnO4
a-CdSnO

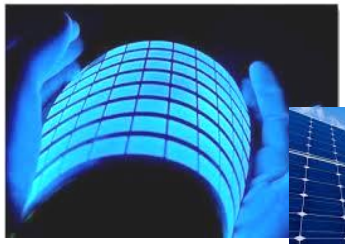
IZO
a-IZO

TiO_2:Nb

ZnO:Al, Zn_2SnO_4,
$ZnSnO_3$, a-ZnSnO

$InGaZnO_4$
a-InGaZnO

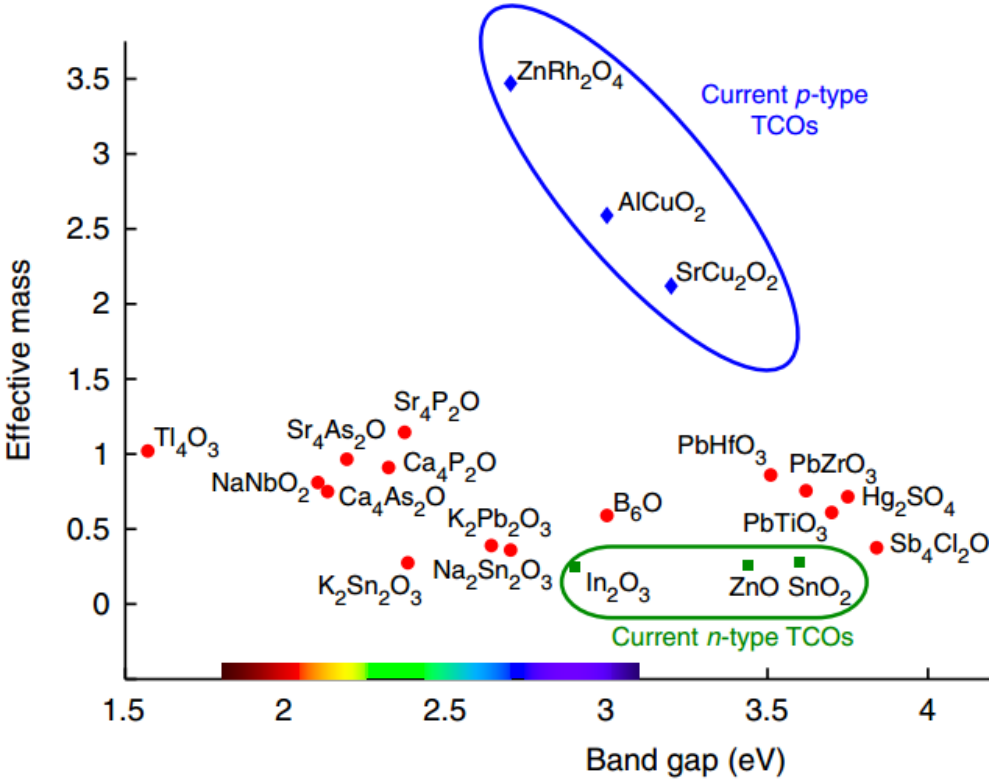
$SrVO_3$
$CaVO_3$

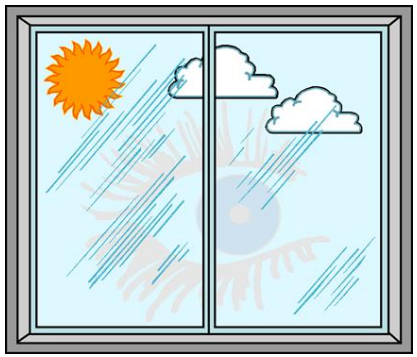


New Generation of TCMs?

Bipolar Doping of TCOs

- Most of the well known post-TM TCOs are n-type. Why?
- How to achieve p-type doping in TCOs?
- Is it possible to have bipolarly dopable TCO?

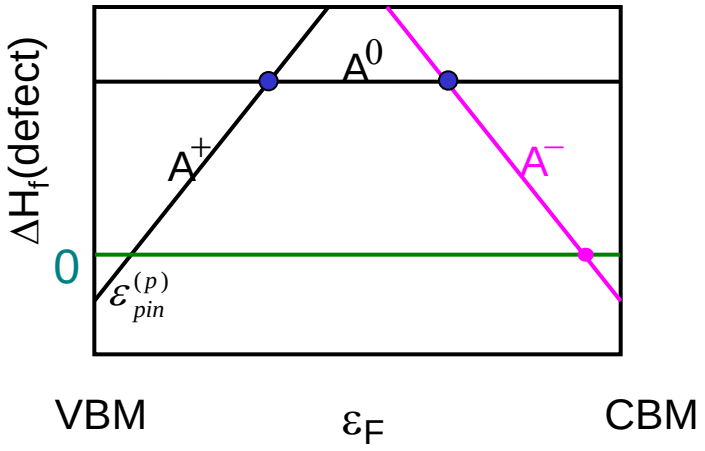




The Doping Limit Rule

The dopability of a material is determined by its band alignment in an absolute energy scale

$$\Delta H^{(\alpha,q)}(E_F,\mu) = \Delta E^{(\alpha,q)}(E_F=0,\mu_i=0) + \Sigma\, n_i\mu_i + qE_F$$



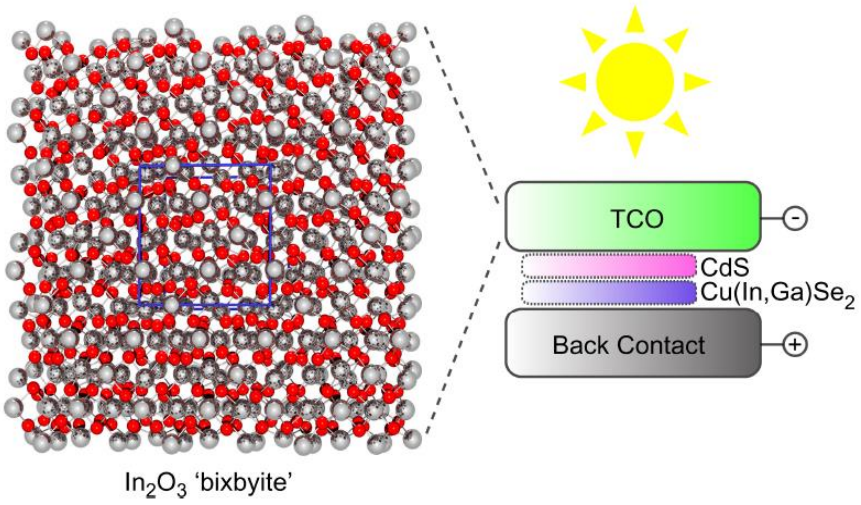
A material is difficult to be doped

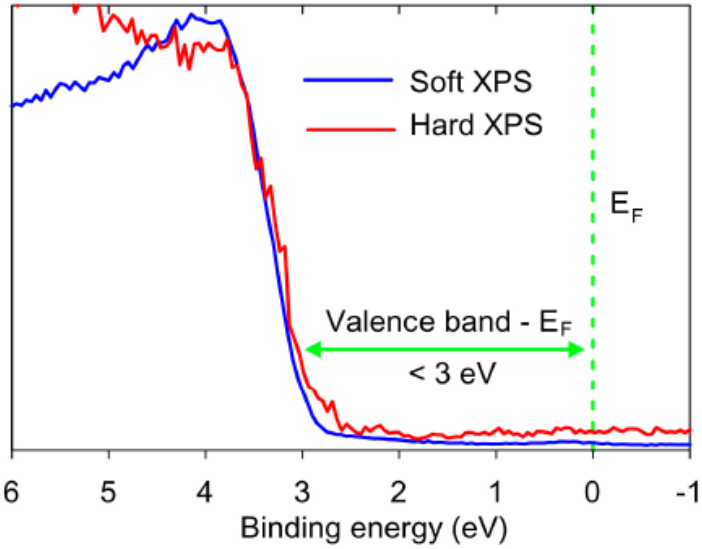
n-type if the CBM is too high

p-type if the VBM is too low

[Zhang, Wei, and Zunger, JAP 83, 3192 (1998)]

Optical Peculiarity of Metal Oxides: In_2O_3

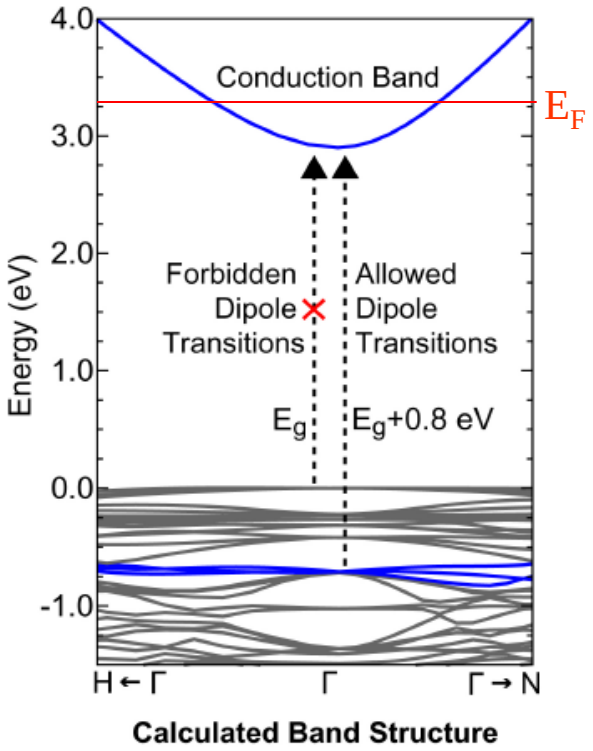




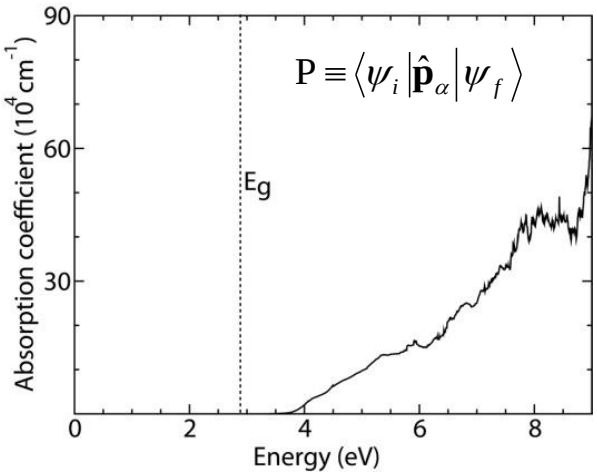
- In_2O_3 doped with Sn (ITO) is currently the best TCO materials. It has an optical band gap of 3.7 eV and high electron mobility (>80 $cm^2\ V^{-1}\ s^{-1}$), thus is widely used in optoelectronic devices.

- However, the band structure of In_2O_3 is not very well understood: Despite its high optical band gap, XPS measurements suggest that its band gap should be less than 3 eV. Does it has an indirect gap?

Why In_2O_3 Is a Good n-type TCO?



Calculated Band Structure



- In_2O_3 has a low CBM due to the large atomic size of In and the low O, s orbital energy, so it can be doped easily n-type

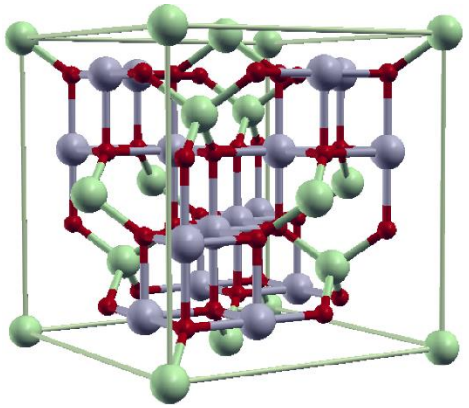
- The fundamental band gap of In_2O_3 is estimated to be

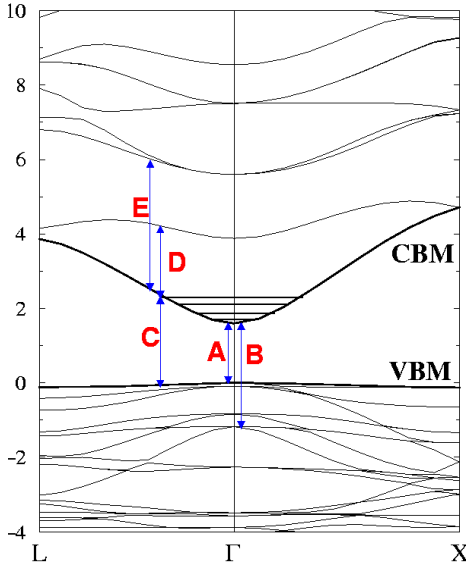
$$E_g \sim 2.9 \text{ eV}$$

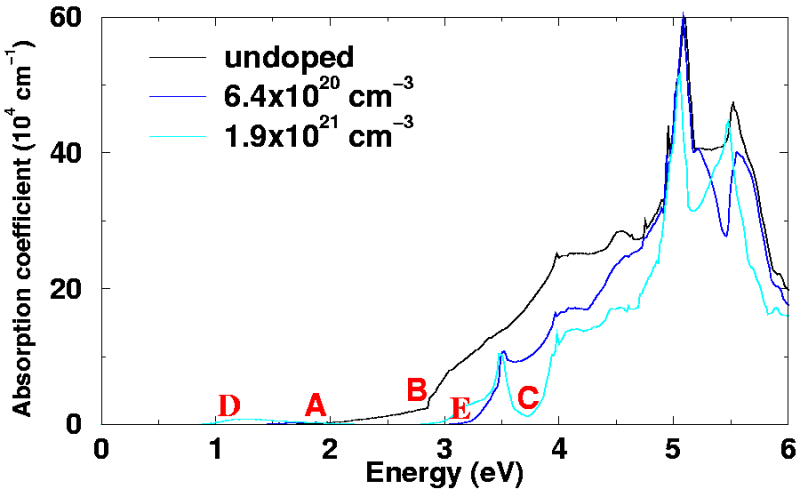
- There exists an disparity between the fundamental band gap (2.9 eV) and the optical band gaps (3.7 eV), i.e., the onset of the optical absorption is 0.8 eV larger than the fundamental band gap so it is transparent to visible light

[A. Walsh, J.F. Da Silva, S.-H. Wei, et al. Phys. Rev. Lett. 100, 167402 (2008).]

Criterion for Being a Good n-type TCO



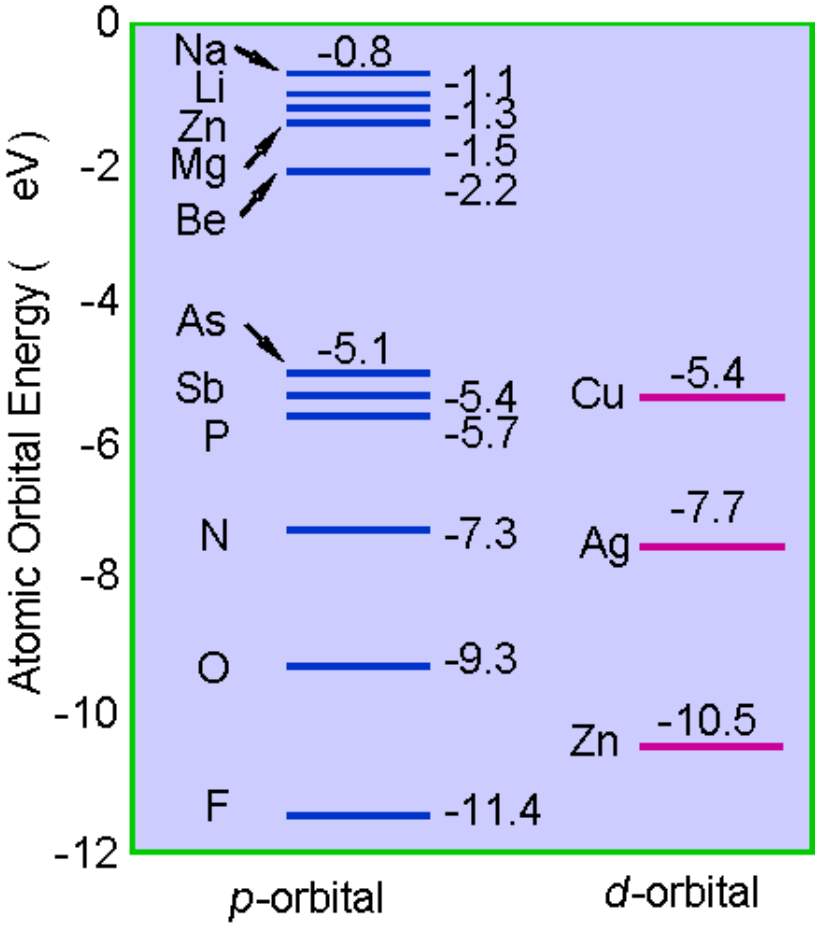




A good n-type TCO should have :

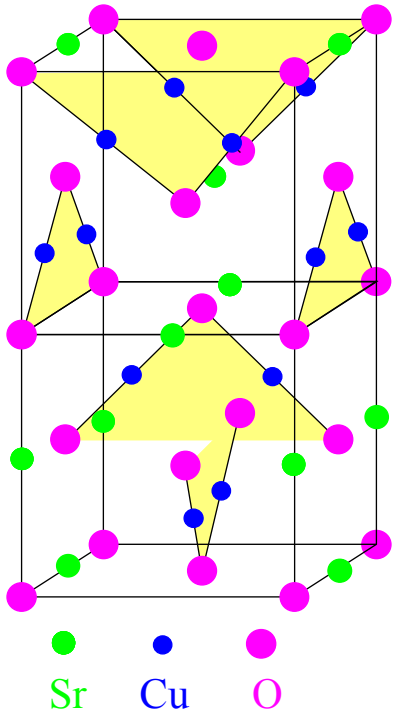
- a small fundamental band gap caused by low CBM (i.e., it should contains large cations)
- a large optical band gap due to forbidden band edge transition (i.e., it should has crystal structure with inversion symmetry and large p-d coupling).
- The separation between first and second CB should be large to avoid intra-band absorption (i.e., material should have large ionicity)

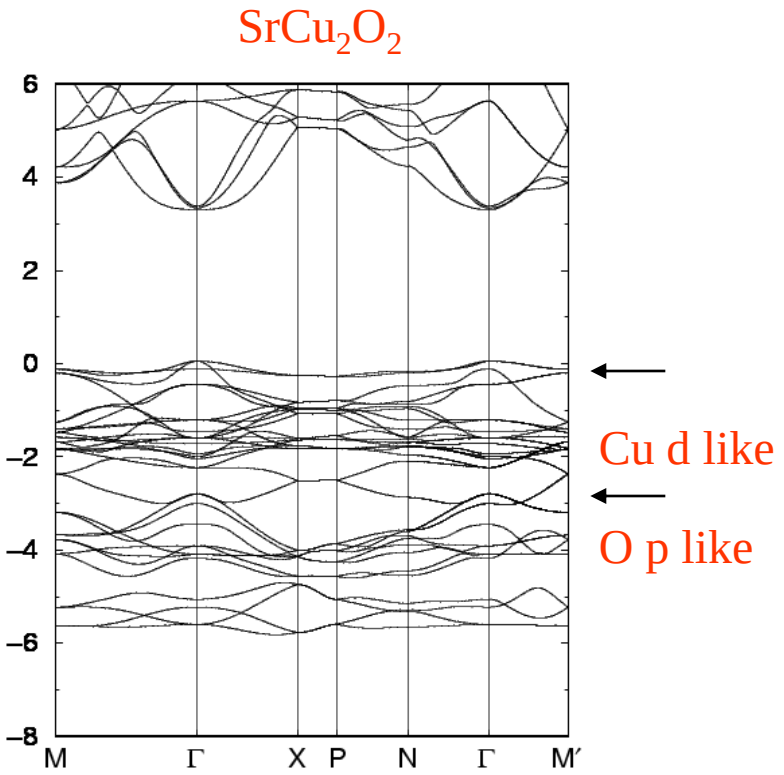
Origin of p-type Doping Difficulty in Oxides



- Oxides are difficult to be doped p-type because their VBMs with O, p character are too low in energy, e.g., there are no group-V element that is more electronegative than O
- p-type TCO can be obtained by increasing the VBM
- A true wide gap transparent material is not possible to be doped both p-type and n-type!

Enhance p-type Doping in Oxides by Introducing Cu

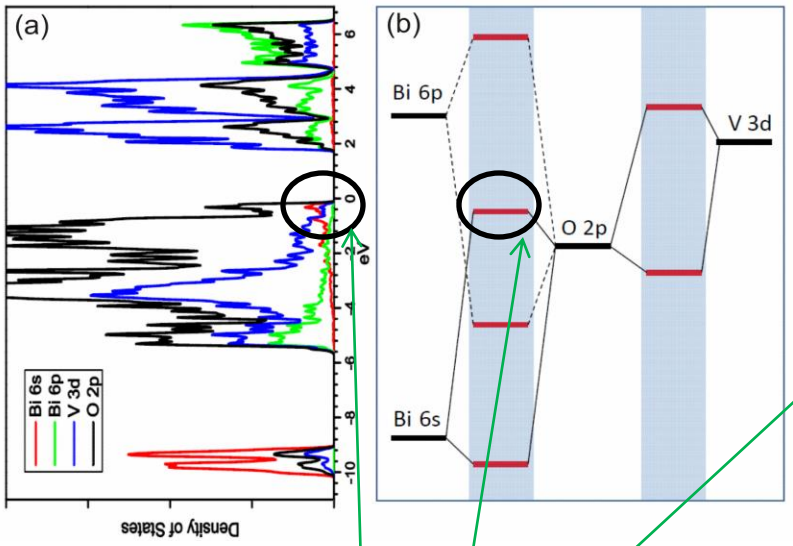


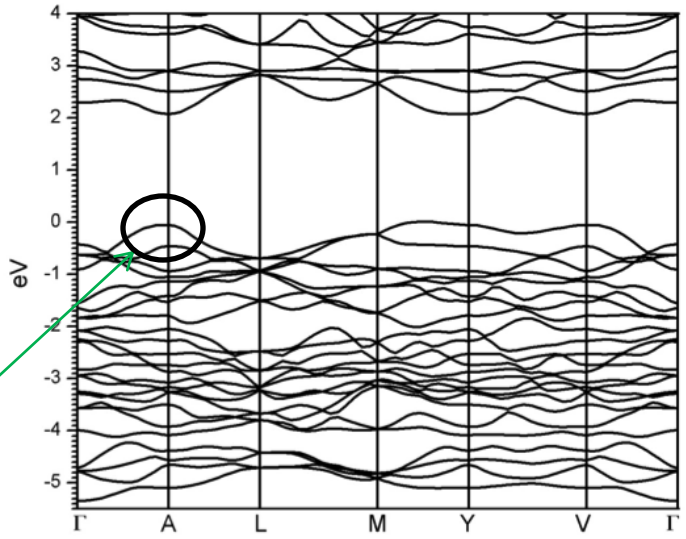


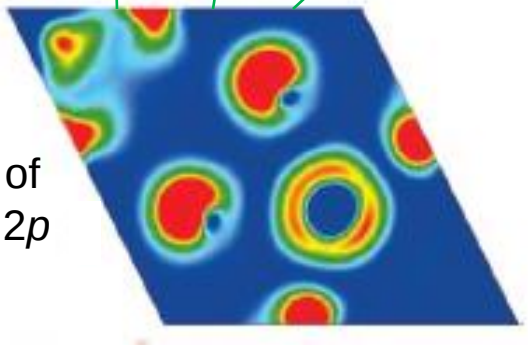
- Cu 3*d* orbital energy is higher than O *p* orbital energy, so the VBM increases
- Coupling between the O *p* and Cu *d* orbitals delocalizes the hole state at the VBM
- Band gap could be tuned by controlling the degree of Cu *d*-*d* coupling

[H. Kawasoe et al., Nature 389, 939 (1997); X. Nie, S. B. Zhang, and S.-H. Wei, Phys. Rev. B **65**, 075111 (2002); X. Nie, S. B. Zhang, and S.-H. Wei, PRL 066405]

Enhance p-type Doping by Introducing Heavy Cations: $BiVO_4$





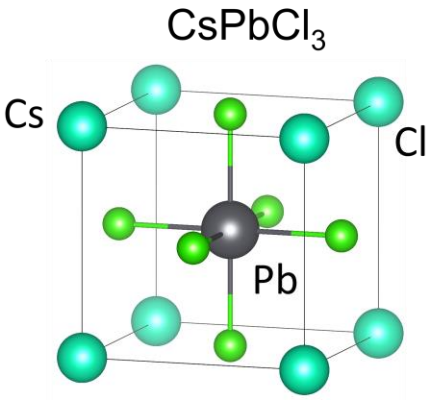


Antibonding of
Bi 6*s* and O 2*p*

Because of the antibonding character of the VBM, p-type doping is easier in $BiVO_4$.

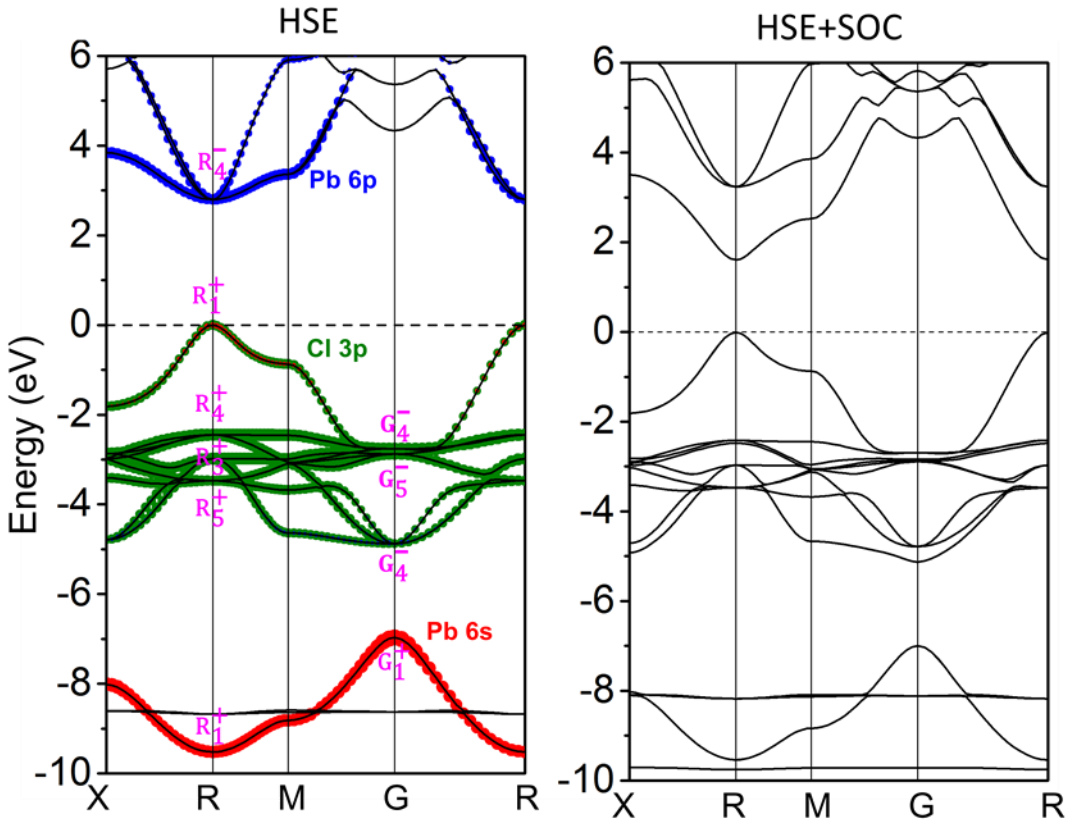
A. Walsh, Y. Yan, M. Huda, M. Mowafak, and S.-H. Wei, *Chem. Mater.* 21, 547(2009)

p-type TCO Based on Perovskite Materials



Merits:

- Band gap: ~3.0 eV
- Optical absorption at R is parity forbidden
- High hole mobility because of s component at VBM
- High-energy VBM because *s-p* repulsion
- Defect properties: easy to dope p-type
- Structural comparability to perovskite solar cell

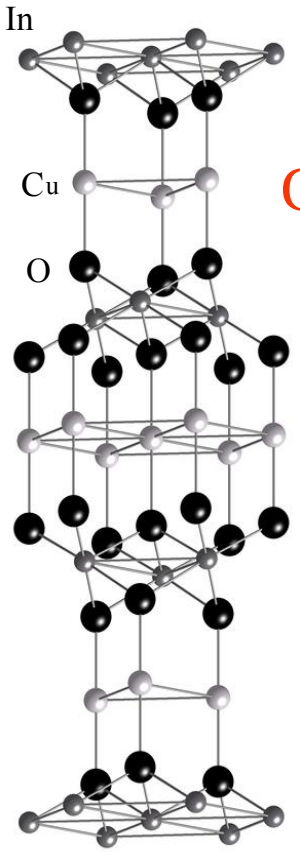


	Calculated	Expt.	
Lattice constant	5.670 A	5.605 A(ICSD)	
Band gap	2.83 eV	3.00 eV	
Effective mass (m/m_0)	X--> R (100)	R--> M (011)	G--> R (111)
	0.164	0.312	0.163

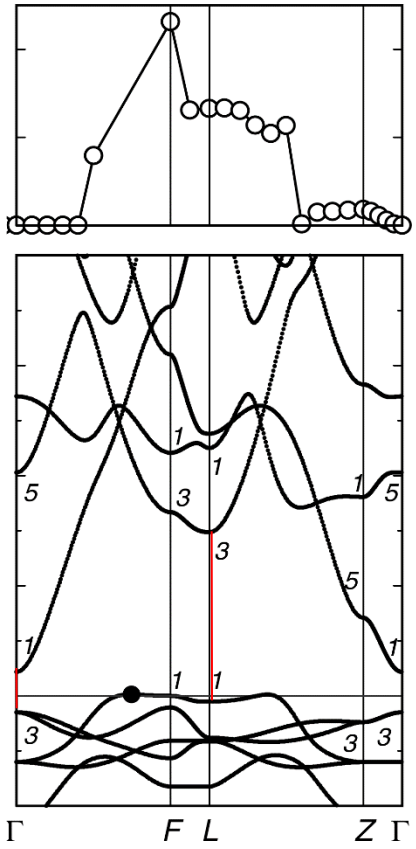
Bipolar Doping of TCOs

- According to the doping limit rule, wide gap transparent material can not be doped both p-type and n-type!
- Is it possible to have bipolarly dopable TCO?

Design Bipolarly Dopable Transparent Conducting Oxides (TCOs)



$CuInO_2$



transition matrix elements

band structure

- A bipolarly dopable TCO should have a large optical band gap so it is transparent, but also a much smaller fundamental band gap so it can be doped both p- and n-type

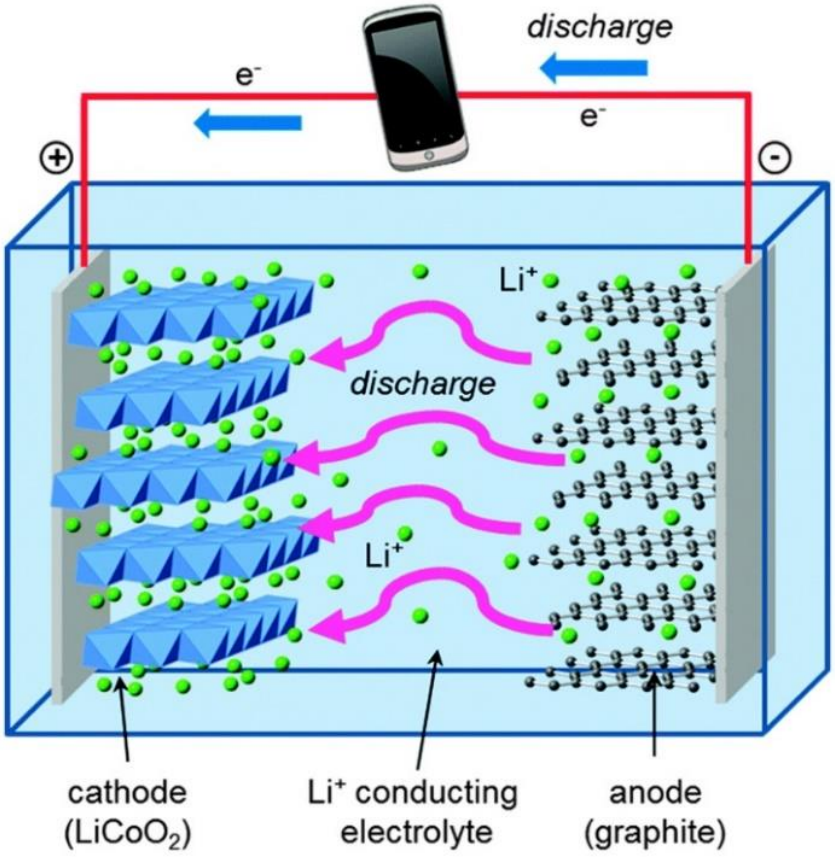
Nie, Wei, Zhang, PRL 88, 066405

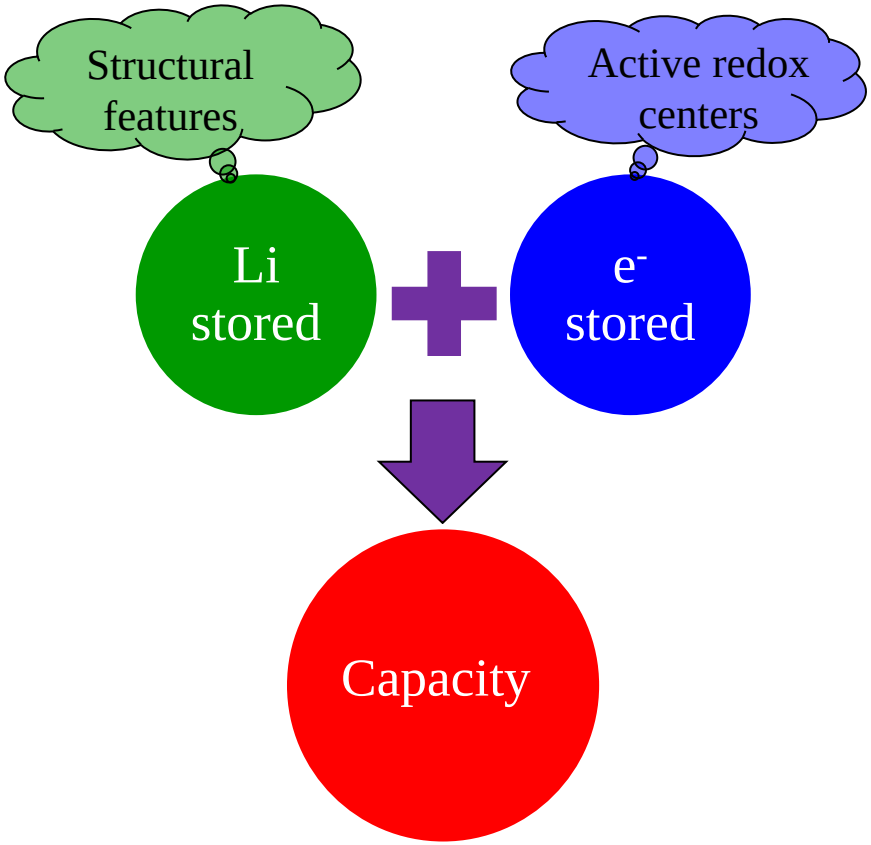
Origin of the Self-limited Energy Density of Oxide Cathode Materials for Li-ion Batteries

LIBs Have Powered the World

But, to reduce the cost, we still need to increase the energy density of LIBs !

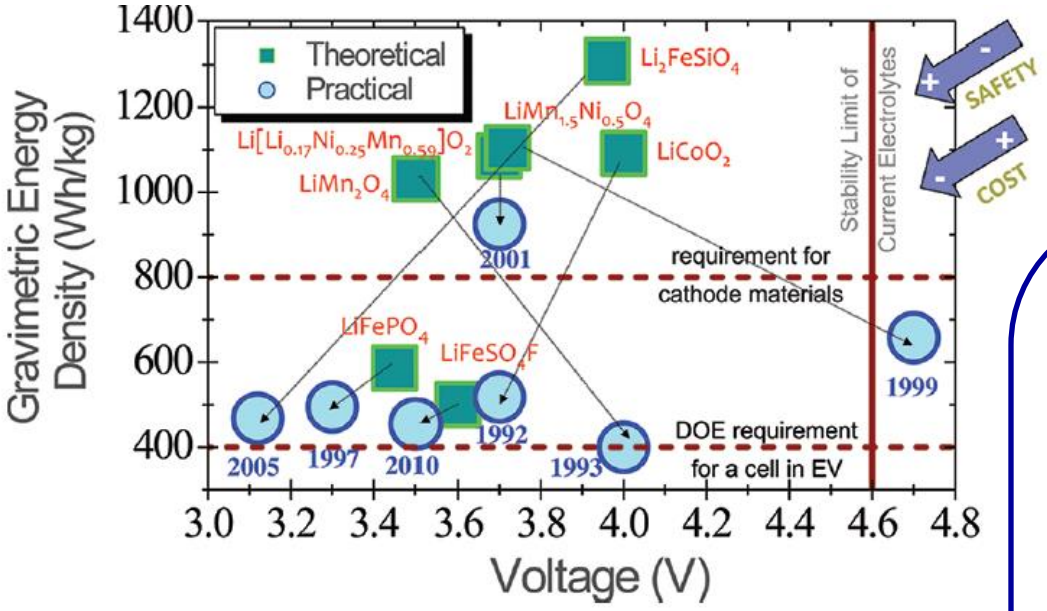
How to Increase the Energy Density of LIBs

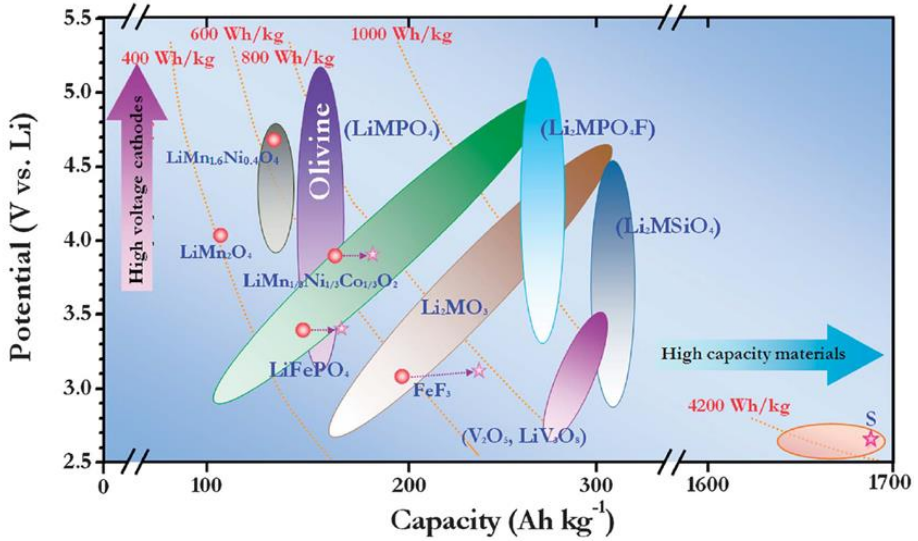




The bottleneck is to increase the capacity of cathode, i.e., the number of Li ions or the number of electrons that can be reversibly exchanged during the delithiation-lithiation process as well as the output voltage.

The Cathode Is the Key





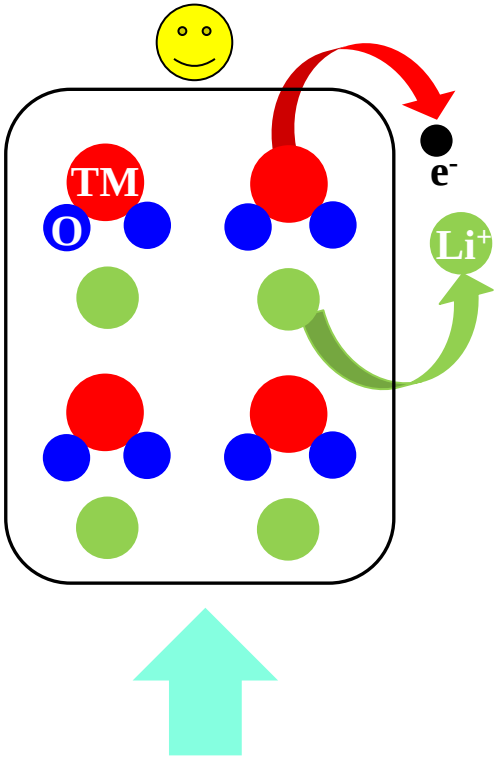
The critical issues for the cathodes:

1. The practical capacity of a cathode is much lower than the theoretical value.
2. What is the fundamental charge-compensation mechanism during electrochemical cycles?
3. What character determines the capacity and stability of a cathode?

Meng et al., Accounts of Chemical Research **1**, 3518 (2013)

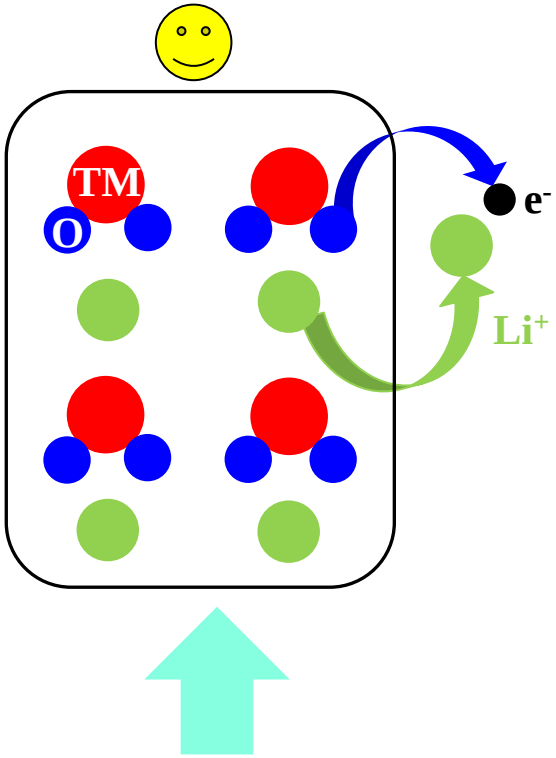
Different Scenarios for the Charge Compensation

Scenario 1:
cationic redox reaction



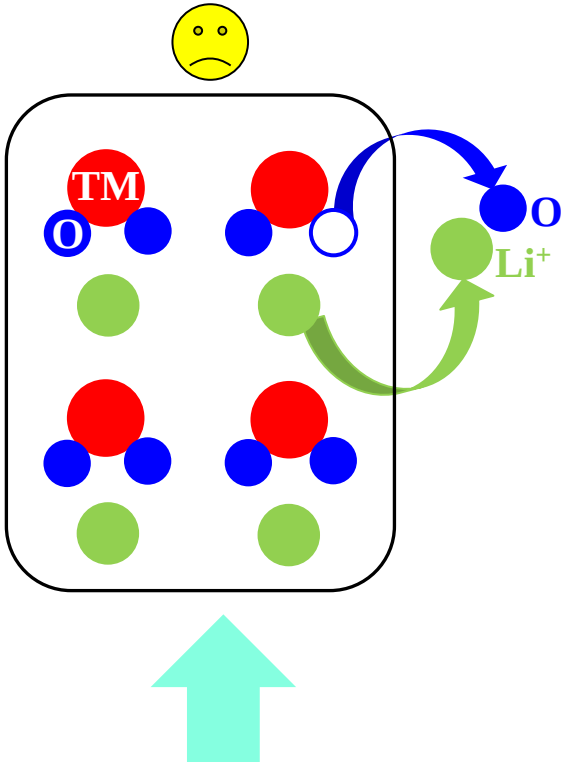
Traditional viewpoint

Scenario 2:
anionic redox reaction



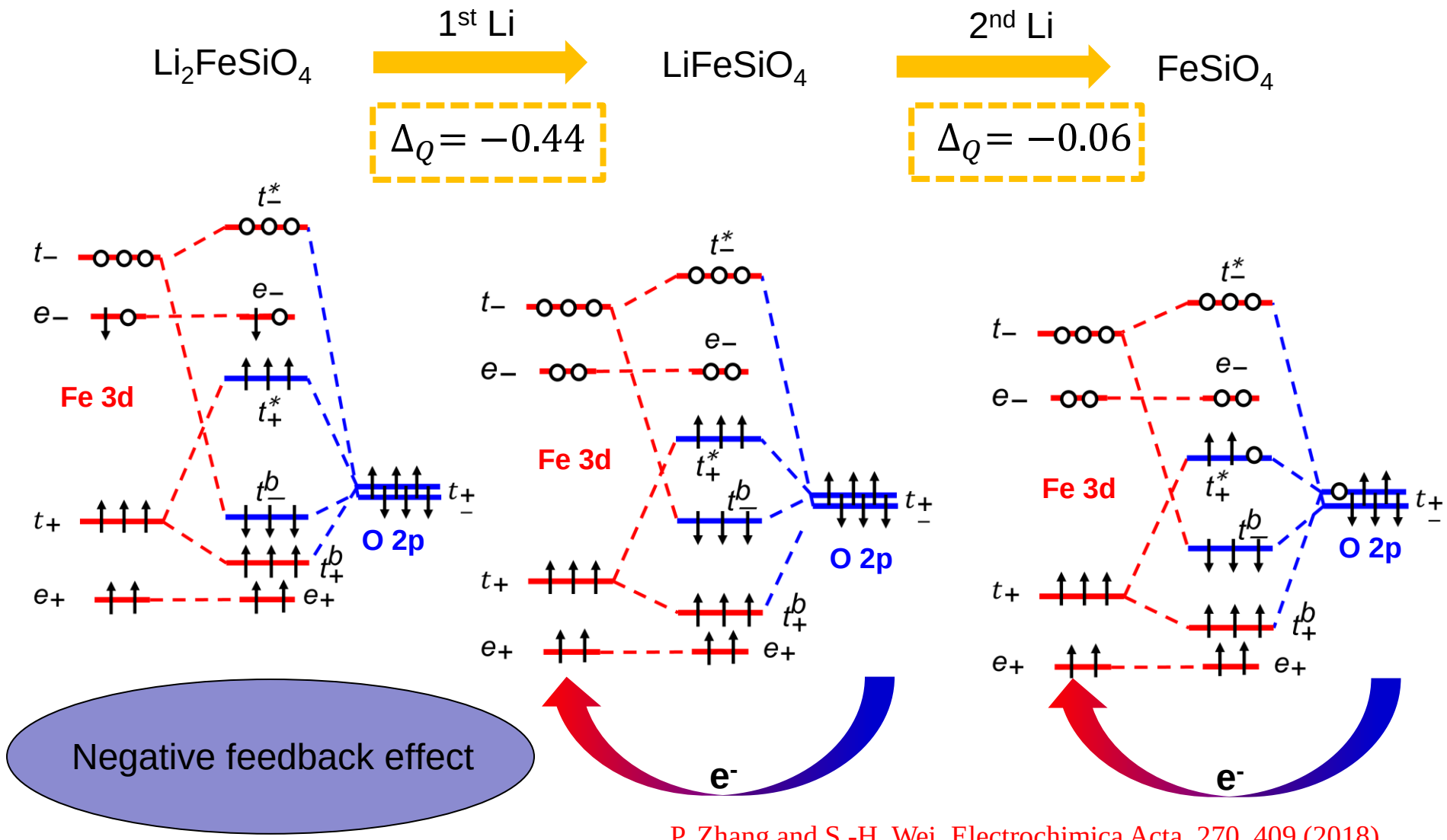
Recently realized

Scenario 3:
anionic vacancy formation



Not well understood

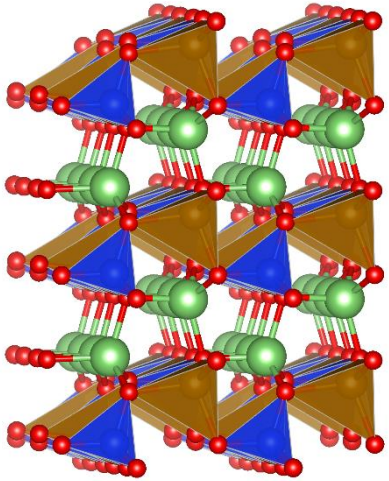
The Charge-compensation Process in Li_xFeSiO_4



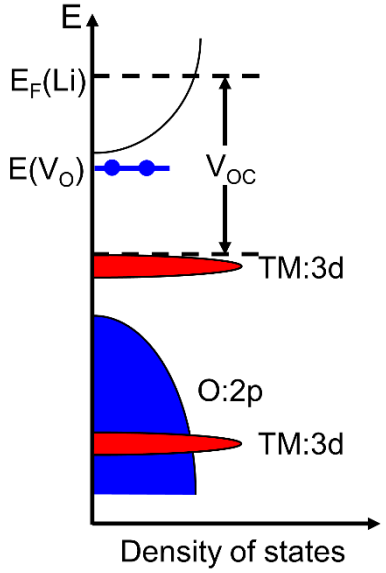
P. Zhang and S.-H. Wei, Electrochimica Acta. 270, 409 (2018).

Mechanism for the Oxygen Vacancy Formation

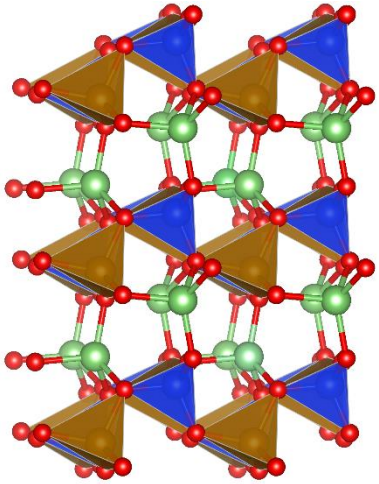
Li_2FeSiO_4



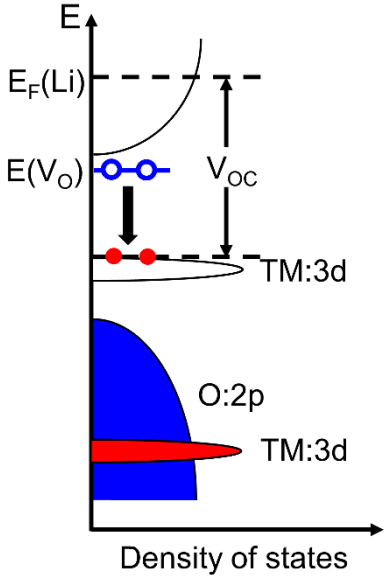
$\Delta H(V_O) = 5.33\ eV$



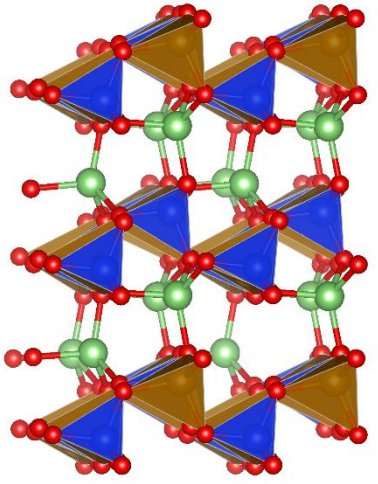
$Li_{2-\delta}FeSiO_4$



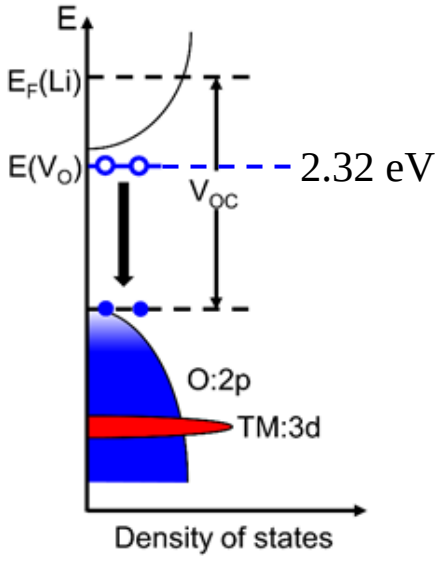
$\Delta H(V_O) = 4.45\ eV$



$Li_{1-\delta}FeSiO_4$

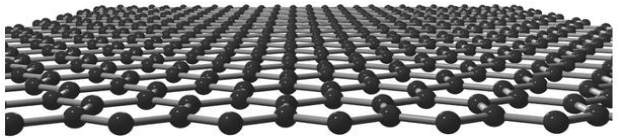


$\Delta H(V_O) = -0.13\ eV$

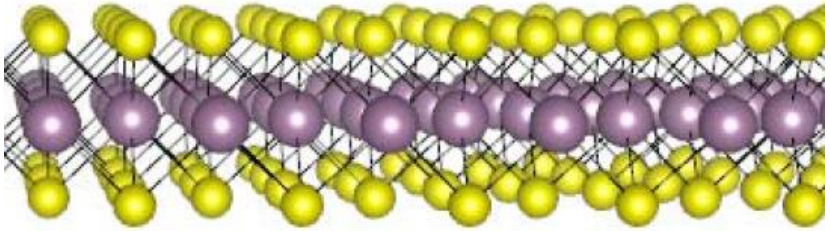


Design 2D Functional Materials Using Atomic Transmutation

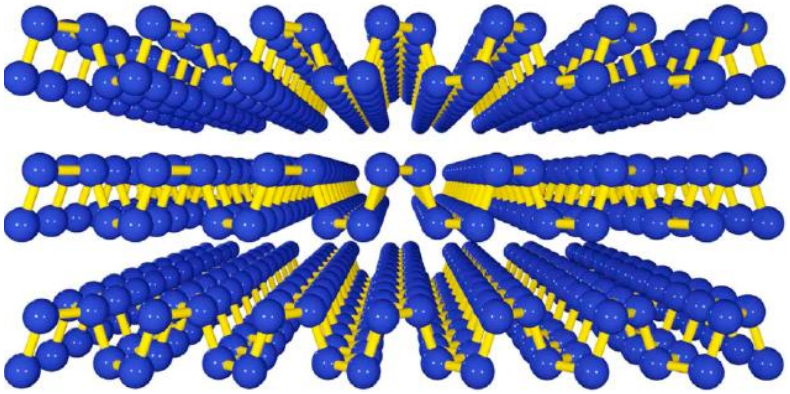
2D Materials



2D semiconductors have many unique structural, electronic and optical properties that is suitable for novel energy-related applications.

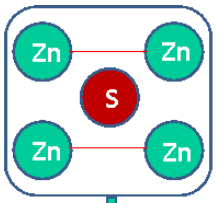


- Mechanically strong
- High thermal conductance
- High electrical mobility at room temperature
- But graphene has no gap, TMD has poor transport property, and phosphorene is unstable

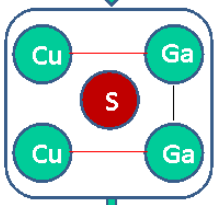


Needs to search/design better 2D materials!

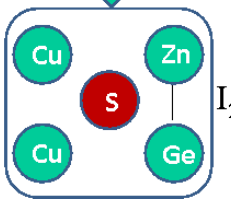
Obtain New Absorber Materials through Atomic Transmutation



II-VI



I-III-VI_2



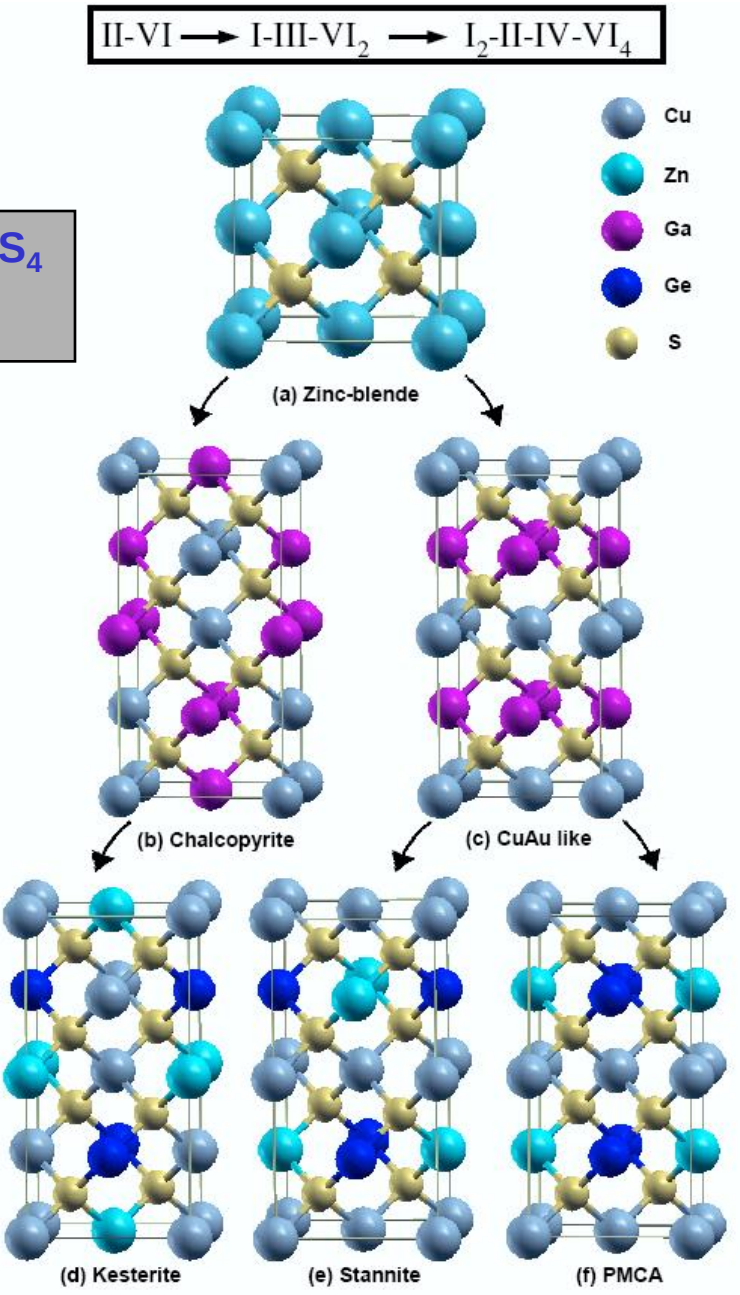
I_2-II-IV-VI_4

$ZnS \rightarrow CuGaS_2 \rightarrow Cu_2ZnGeS_4$

$Cu_2GaInS_4 \rightarrow Cu_2ZnSnS_4$

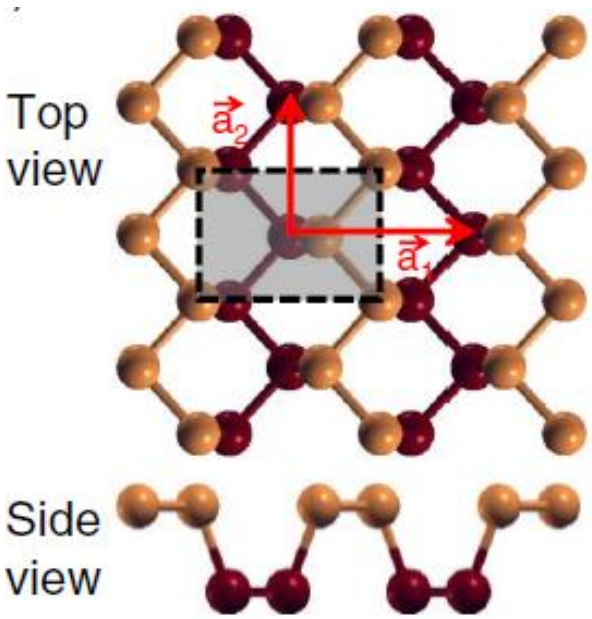
The octet rule

		13 $^2P^o_{1/2}$ **Al** Aluminum 26.981538 $[Ne]3s^23p$ 5.9858	14 $^3P_0$ **Si** Silicon 28.0855 $[Ne]3s^23p^2$ 8.1517	15 $^4S^o_{3/2}$ **P** Phosphorus 30.973761 $[Ne]3s^23p^3$ 10.4867	16 $^3P_2$ **S** Sulfur 32.065 $[Ne]3s^23p^4$ 10.3600
29 $^2S_{1/2}$ **Cu** Copper 63.546 $[Ar]3d^{10}4s$ 7.7264	30 $^1S_0$ **Zn** Zinc 65.409 $[Ar]3d^{10}4s^2$ 9.3942	31 $^2P^o_{1/2}$ **Ga** Gallium 69.723 $[Ar]3d^{10}4s^24p$ 5.9993	32 $^3P_0$ **Ge** Germanium 72.64 $[Ar]3d^{10}4s^24p^2$ 7.8994	33 $^4S^o_{3/2}$ **As** Arsenic 74.92160 $[Ar]3d^{10}4s^24p^3$ 9.7886	34 $^3P_2$ **Se** Selenium 78.96 $[Ar]3d^{10}4s^24p^4$ 9.7524
47 $^2S_{1/2}$ **Ag** Silver 107.8682 $[Kr]4d^{10}5s$ 7.5762	48 $^1S_0$ **Cd** Cadmium 112.411 $[Kr]4d^{10}5s^2$ 8.9938	49 $^2P^o_{1/2}$ **In** Indium 114.818 $[Kr]4d^{10}5s^25p$ 5.7864	50 $^3P_0$ **Sn** Tin 118.710 $[Kr]4d^{10}5s^25p^2$ 7.3439	51 $^4S^o_{3/2}$ **Sb** Antimony 121.760 $[Kr]4d^{10}5s^25p^3$ 8.6084	52 $^3P_2$ **Te** Tellurium 127.60 $[Kr]4d^{10}5s^25p^4$ 9.0096

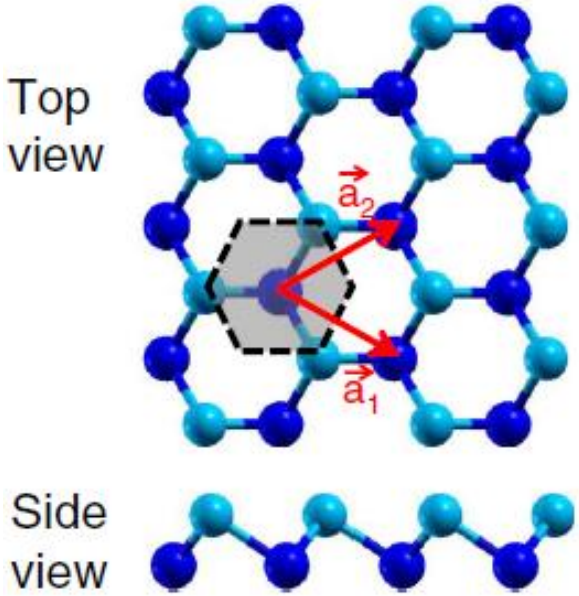


Phosphorene ⟶ SiS

Black phosphorene



Blue phosphorene



11 IB	12 IIB	13 $^2P^\circ_{1/2}$ **Al** Aluminum 26.981538 $[Ne]3s^23p$ 5.9858	14 $^3P_0$ **Si** Silicon 28.0855 $[Ne]3s^23p^2$ 8.1517	15 $^4S^\circ_{3/2}$ **P** Phosphorus 30.973761 $[Ne]3s^23p^3$ 10.4867	16 $^3P_2$ **S** Sulfur 32.065 $[Ne]3s^23p^4$ 10.3600
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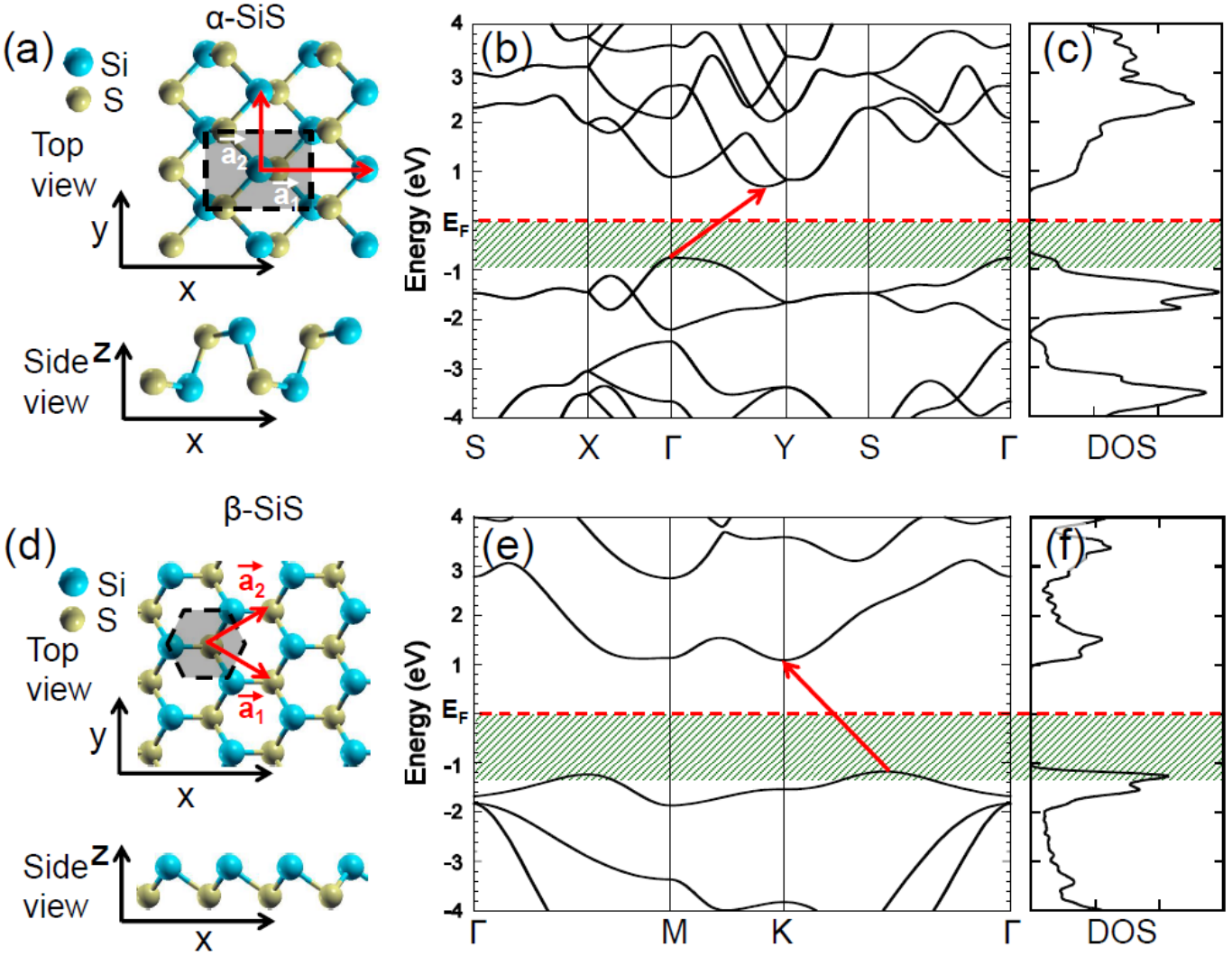
47 $^2S_{1/2}$ **Ag** Silver 107.8682 $[Kr]4d^{10}5s$ 7.5762	48 $^1S_0$ **Cd** Cadmium 112.411 $[Kr]4d^{10}5s^2$ 8.9938	49 $^2P^\circ_{1/2}$ **In** Indium 114.818 $[Kr]4d^{10}5s^25p$ 5.7864	50 $^3P_0$ **Sn** Tin 118.710 $[Kr]4d^{10}5s^25p^2$ 7.3439	51 $^4S^\circ_{3/2}$ **Sb** Antimony 121.760 $[Kr]4d^{10}5s^25p^3$ 8.6084	52 $^3P_2$ **Te** Tellurium 127.60 $[Kr]4d^{10}5s^25p^4$ 9.0096

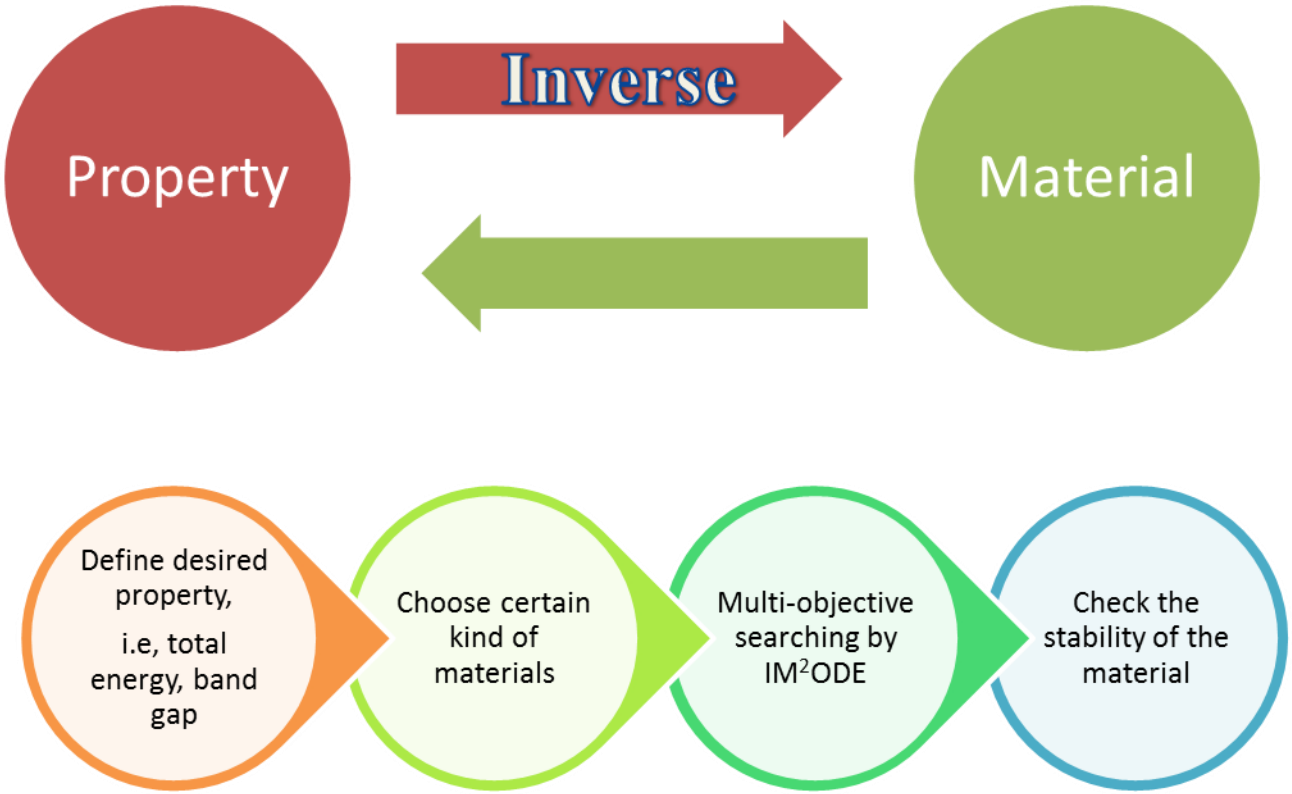
Atomic Transmutation for 2D Materials: Does it work?



Z. Zhu, J. Guan, D. Liu, D. Tománek, *ACS Nano* **9**, 8284 (2015).

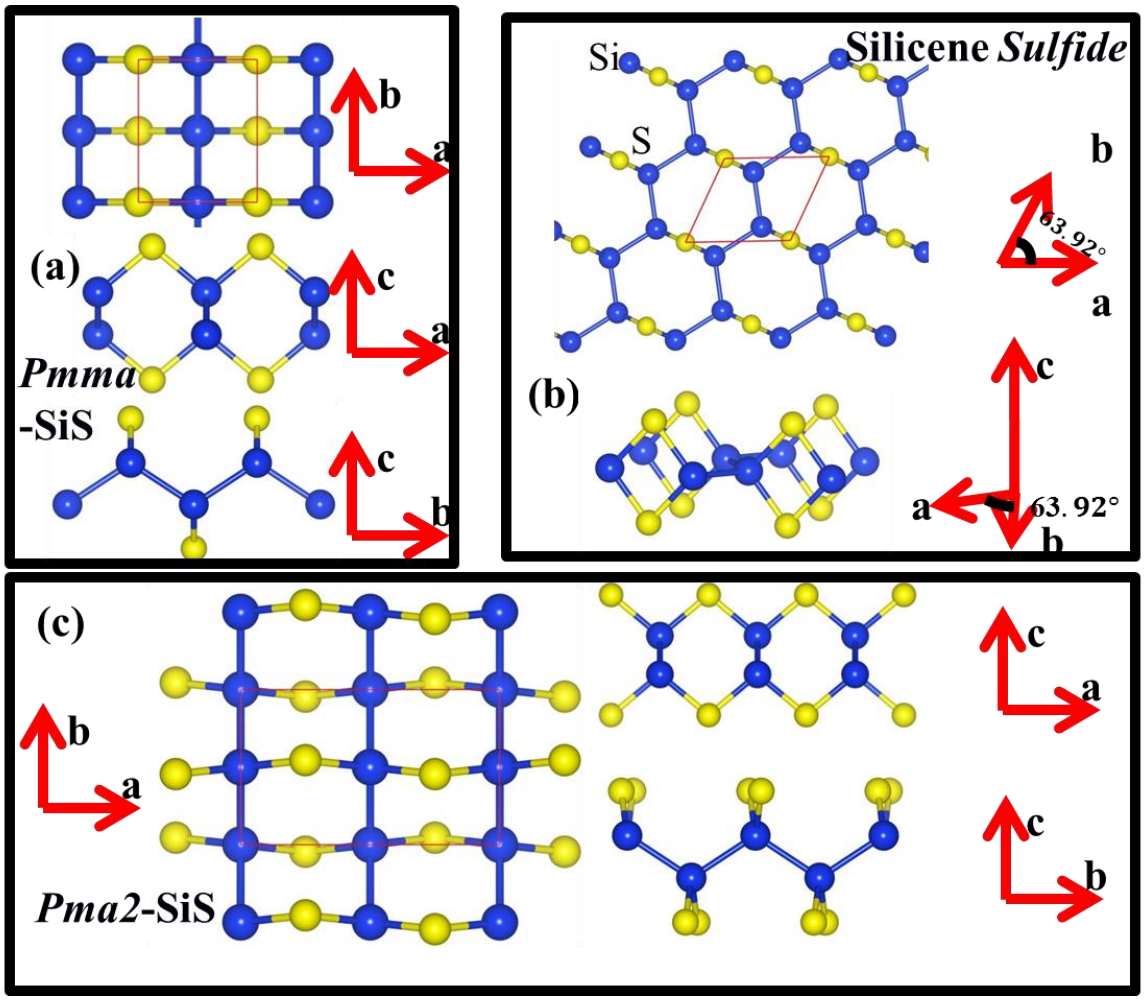
IM^{2}ODE

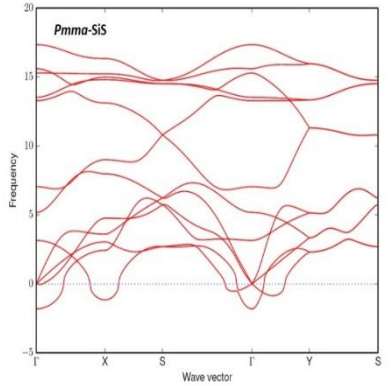
Inverse-design of Materials by Multi-Objective Differential Evolution

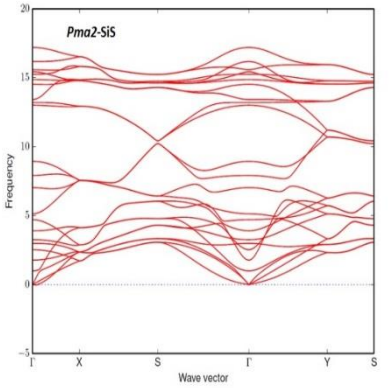


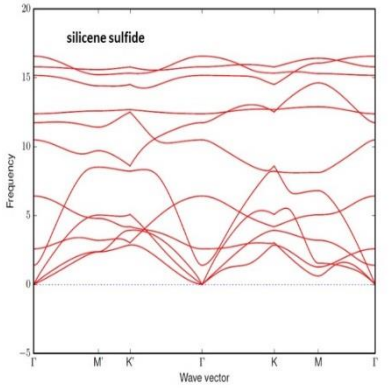
Zhang, Y.-Y.; Gao, W.; Chen, S.; Xiang, H.; Gong, X.-G. *Comput. Mater. Sci.* **2015**, 98, 51.

The Lowest Energy Structures of SiS Systems



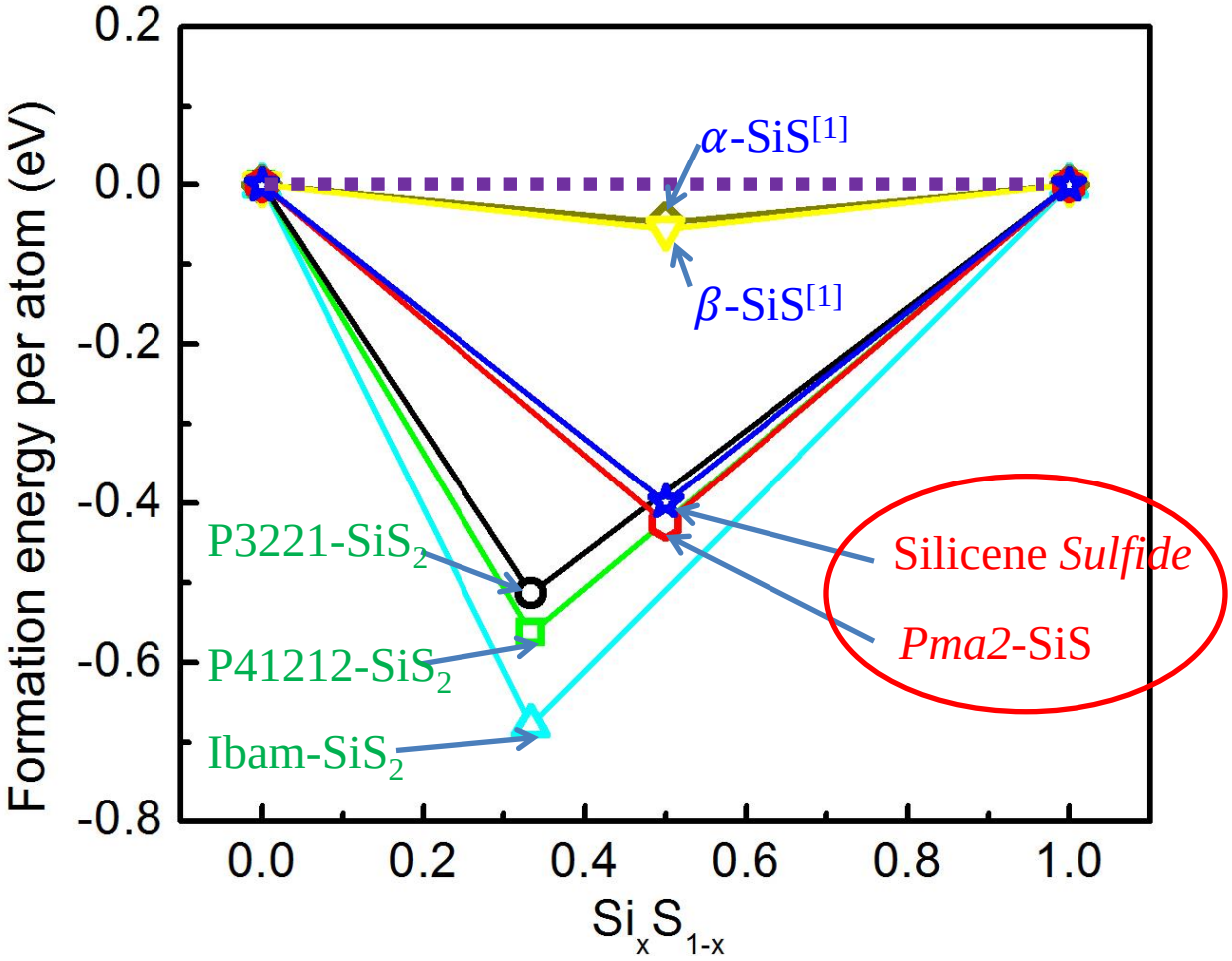






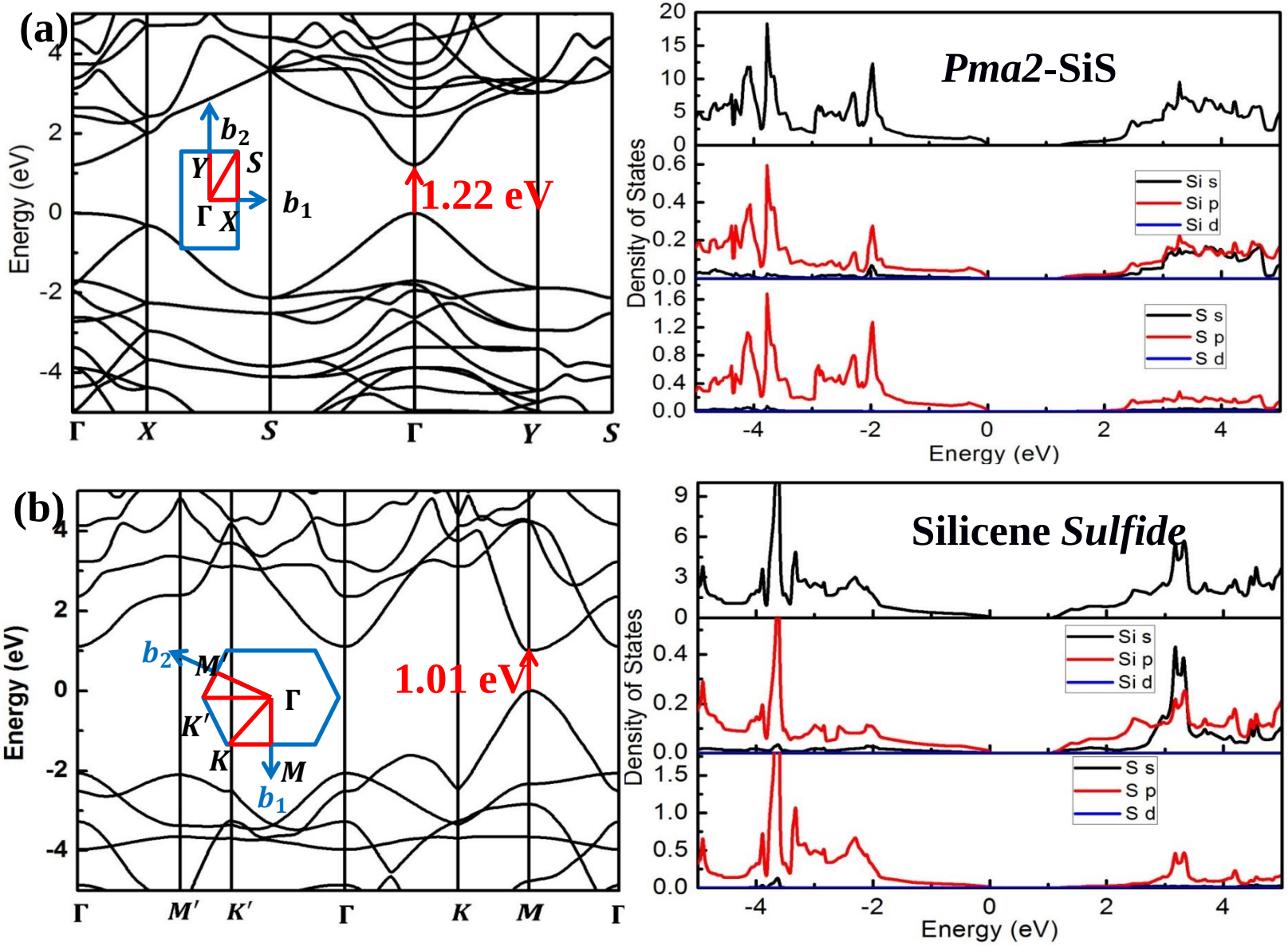
J.-H. Yang, Y. Zhang, W.-J. Yin, X. G. Gong, B. I. Yakobson, and S.-H. Wei, Nano Lett. **16**, 1110 (2016).

Formation Energy Diagram of Si_xS_{1-x}

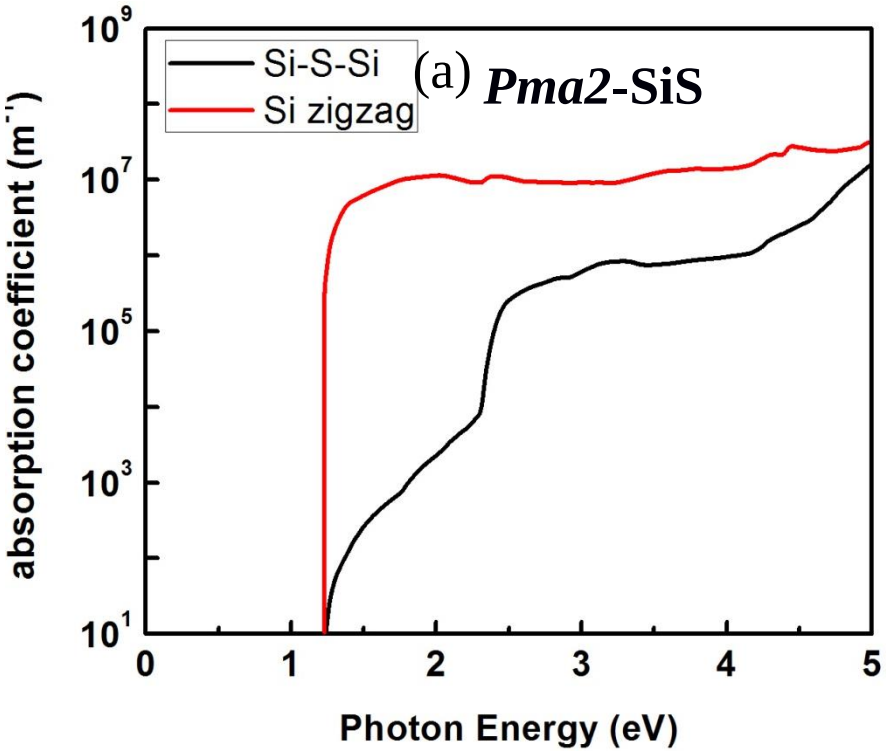


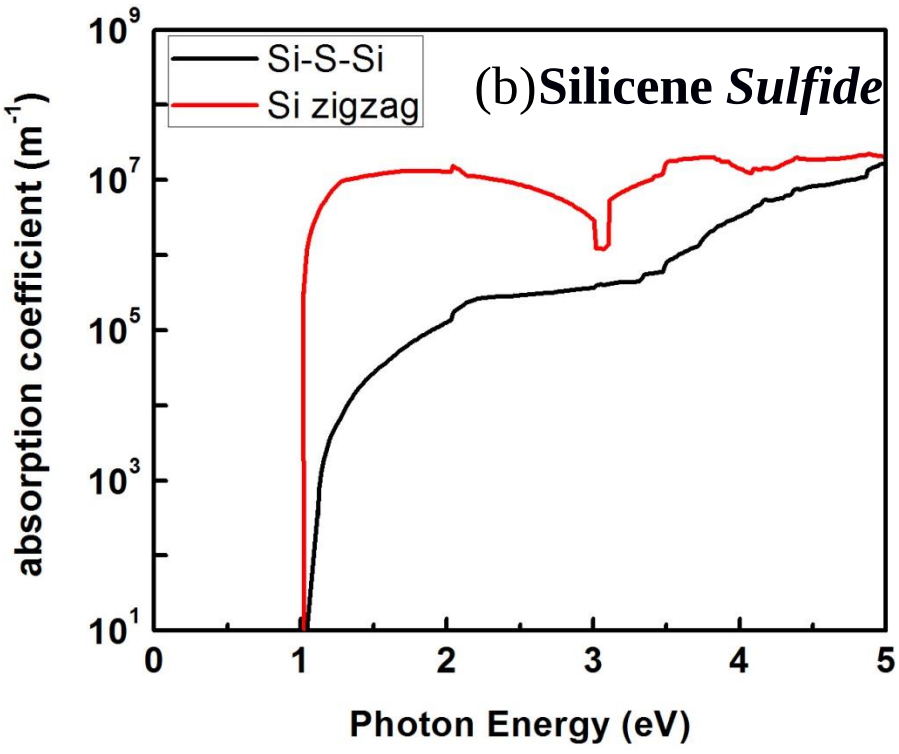
- [1] Z. Zhu, *ACS Nano* **9**, 8284 (2015).
- SiS_2 structures are the most stable 3D structure

Band Structures and DOS

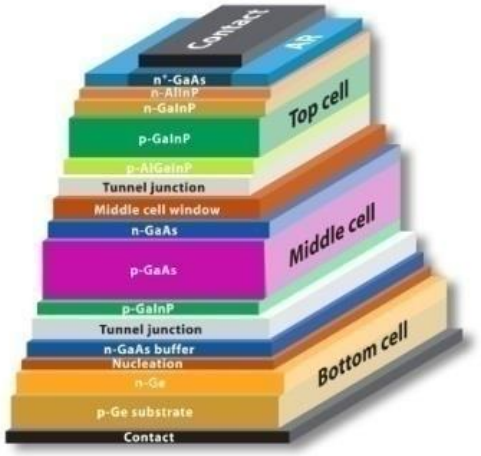


Optical Properties



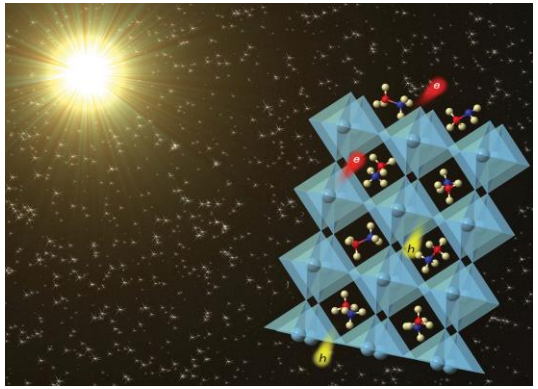


Both Pma2-SiS and Silicene Sulfide have direct bandgaps which can allow optical transitions at band edges and have values close to the optimal requirement for solar cell applications. It can also be used as sensor for polarized light.



Summary

First-principles electronic structure calculations can provide deep physical understanding on the material properties. Recent development in first-principles theory and computational power has enabled us to perform ab initio knowledge-based material design. It has now become a vital tool for accelerating scientific discovery of new energy materials.



Collaborators:

Wanjian Yin
Jihui Yang
Huixiong Deng
Peng Zhang
Jingxiu Yang
Lijun Zhang






Thank You for your attention

Members of Materials and Energy Division

Division Head

Suhuai Wei

Chair Prof.

Shiwu Gao

Assist. Prof.

Bing Huang

Assist. Prof.

Pengfei Guan

Res. Assist. Prof.

Shuxian Hu

Admin. Assist.

Yi Feng

研究部人员构成及研究方向

Roberto Car

Quantum and statistical mechanics. New method development based on ab-initio molecular dynamics simulation and density functional theory (DFT).

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学习经历：

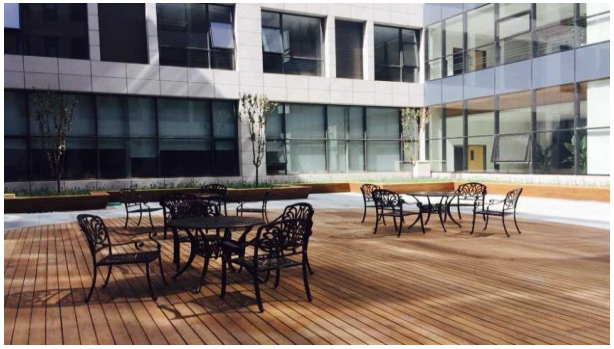
- 2009/09-2014/07： 中国科学院半导体研究所凝聚态物理专业，获理学博士学位
  导师：李京波研究员
- 2005/09-2009/07： 厦门大学物理系微电子学专业，获理学学士学位

工作经历：

- 2015/11-目前: 美国劳伦斯伯克利国家实验室材料学部，博士后
  合作导师：Lin-Wang Wang 研究员
- 2014/10 -2015/09: 比利时安特卫普大学物理系，FWO Pegasus Marie-Curie 博士后
  合作导师：欧洲科学院院士 Francois M. Peeters 教授

CSRC

Entrance Hall



Court Yard

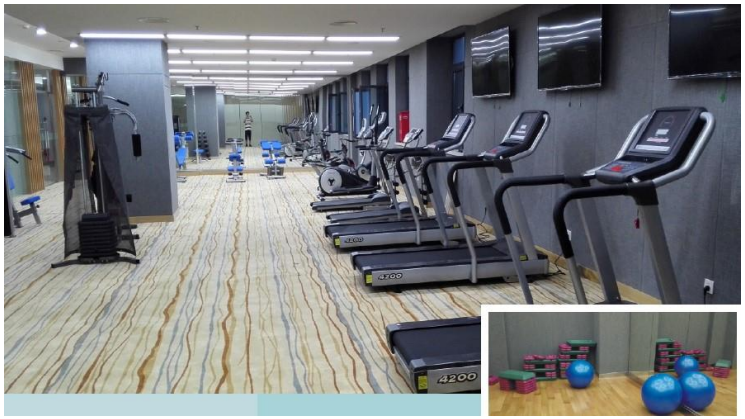
Academic Hall

Conference Room

CSRC

Cafeteria

Drinking Bar



Exercise Room

Ping-Pong Room