



Passivating the Grain Boundaries in CdTe: A First-principles Study

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- **1 Background**
- **2 Simulations on CdTe GBs**
- **3 Conclusion**



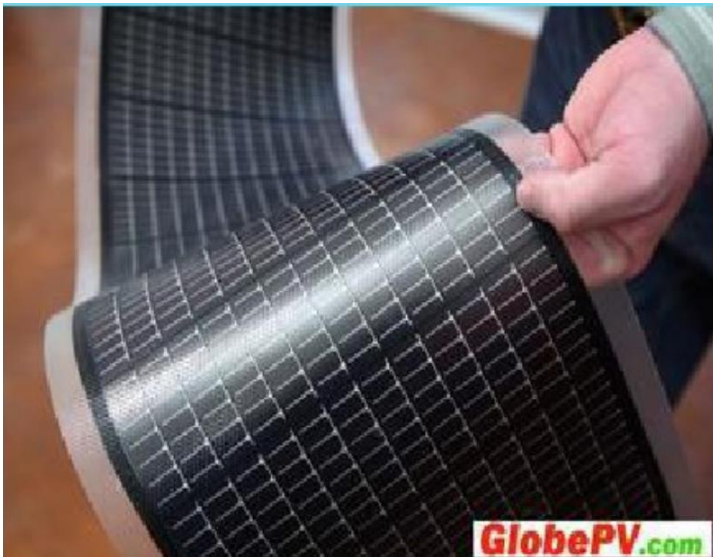
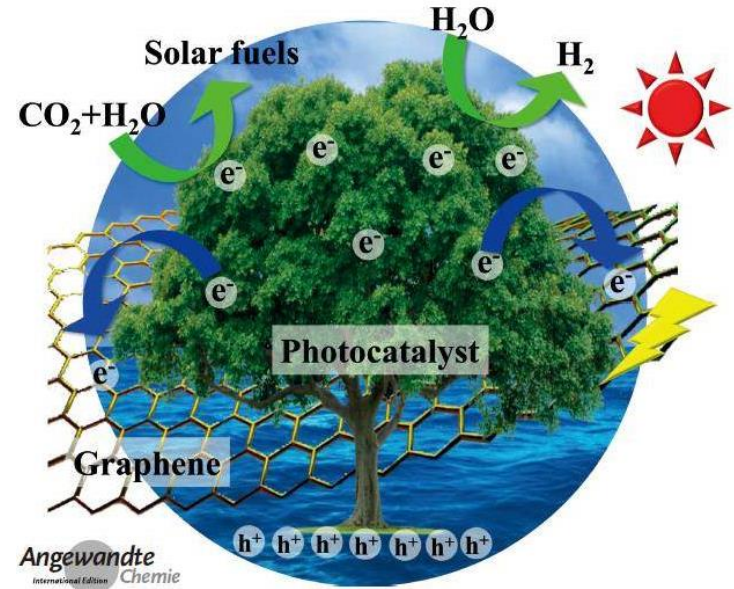
Background

Humanity's Top Ten Problems for next 50 years

1. ENERGY
2. WATER
3. FOOD
4. ENVIRONMENT
5. POVERTY
6. TERRORISM & WAR
7. DISEASE
8. EDUCATION
9. DEMOCRACY
10. POPULATION



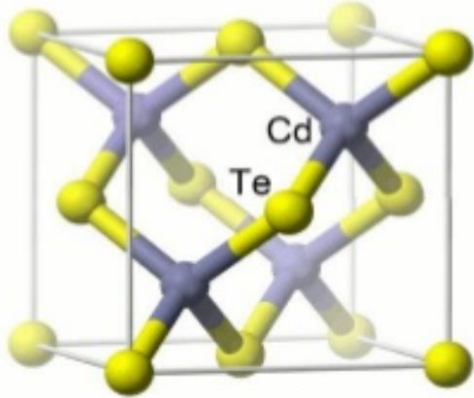
2003	6.3	Billion People
2050	8-10	Billion People





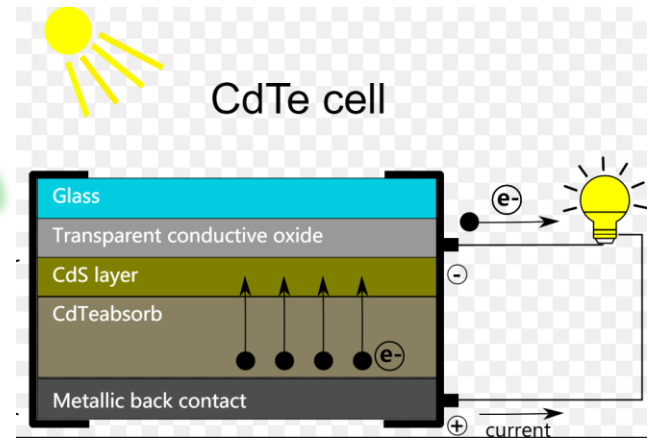
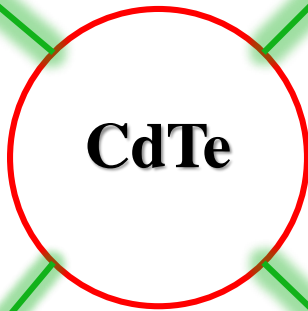
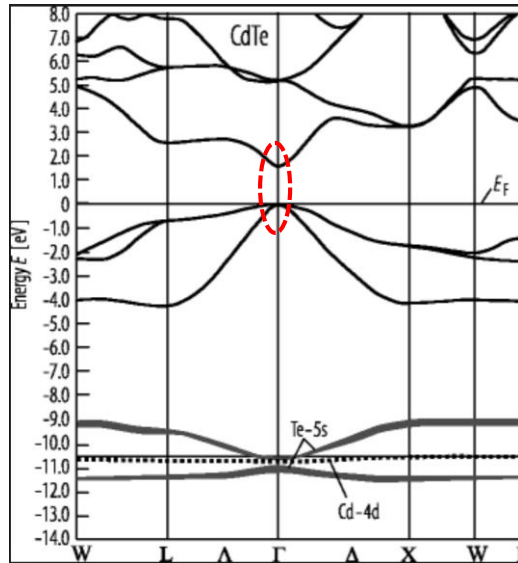
CdTe

Zinc Blende



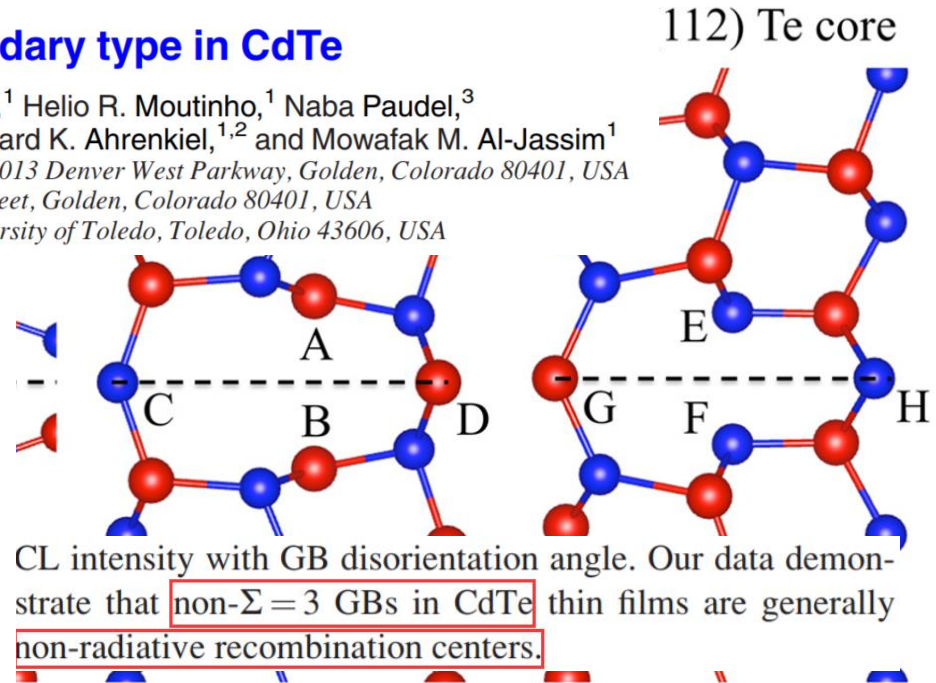
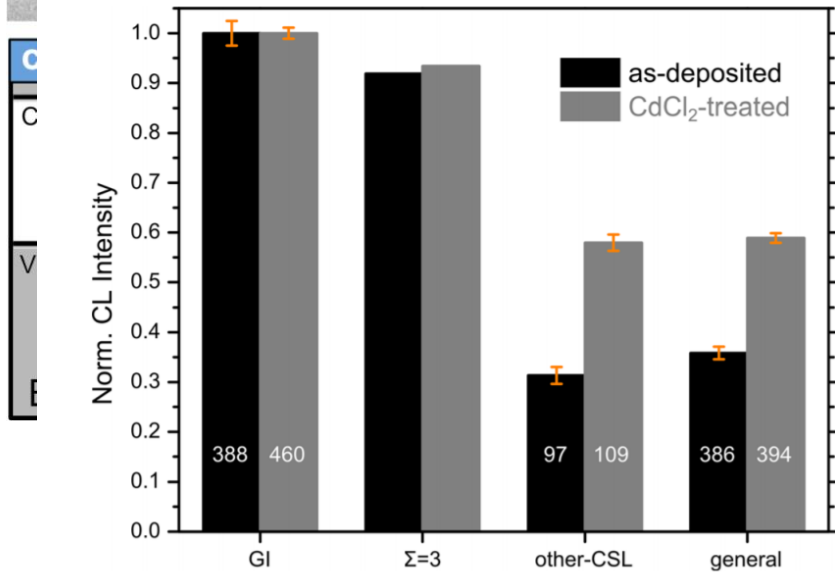
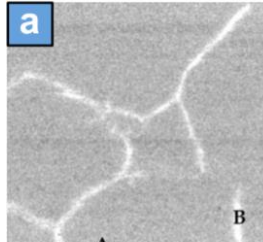
Lattice Constants	$a=b=c=6.48 \text{ \AA}$
Band-gap	1.45~1.55 eV

Band Structure



Recombination by grain-boundary type in CdTe

John Moseley,^{1,2,a)} Wyatt K. Metzger,¹ Helio R. Moutinho,¹ Naba Paudel,³ Harvey L. Guthrey,¹ Yanfa Yan,³ Richard K. Ahrenkiel,^{1,2} and Mowafak M. Al-Jassim¹
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FIG. 4. Bar chart showing the average CL intensity calculated for each of the GB types, including $\Sigma = 3$, other-CSL, and general GBs relative to the average GI CL intensity for the as-deposited and CdCl₂-treated films. The numbers at the bottom of the bars indicate the number of GBs sampled of each type. The orange brackets at the top of the bars give the estimated uncertainty in the averages.

would introduce **trapping states** and however, GBs in CdTe showed efficient It probably stems from the impurities



Dopants in CdTe

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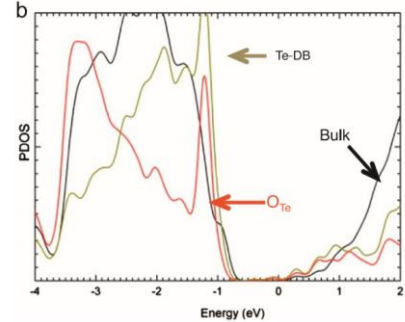
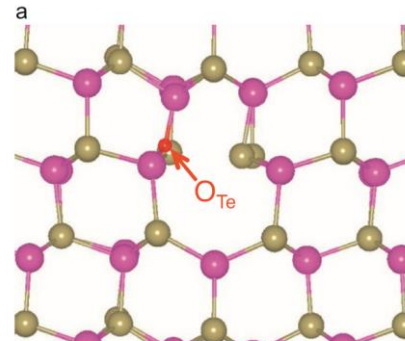
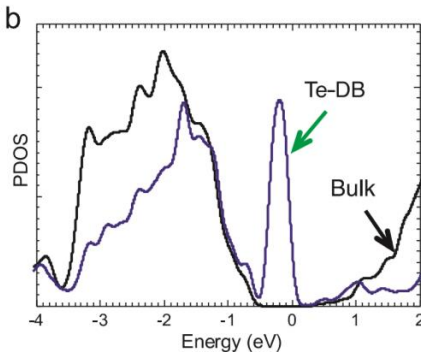
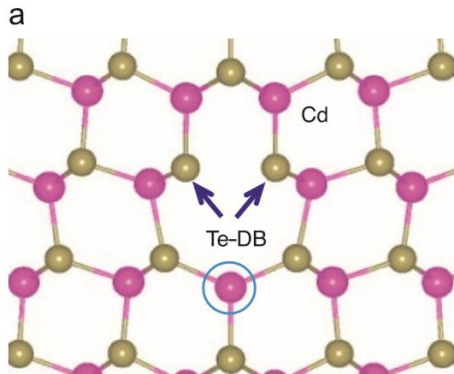
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Possible effects of oxygen in Te-rich $\Sigma 3$ (112) grain boundaries in CdTe

Chunbao Feng^{a,b,c}, Wan-Jian Yin^d, Jinlan Nie^a, Xiaotao Zu^a, Muhammad N. Huda^b, Su-Huai Wei^c, Mowafak M. Al-Jassim^c, Yanfa Yan^{d,*}

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polycrystalline CdTe

and Su-Huai Wei^{1,3,a}

doi:10.1088/0268-1242/31/9/093001



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thin film solar

University of Liverpool, Liverpool,



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Approach: Density Functional Theory (DFT)

Software: VASP

Functional: PBE, HSE06 (for some SCF calculations)



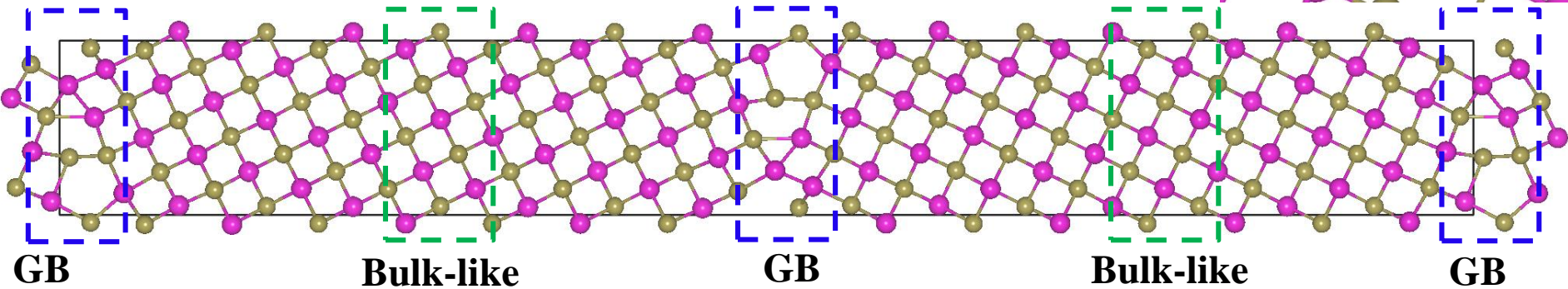
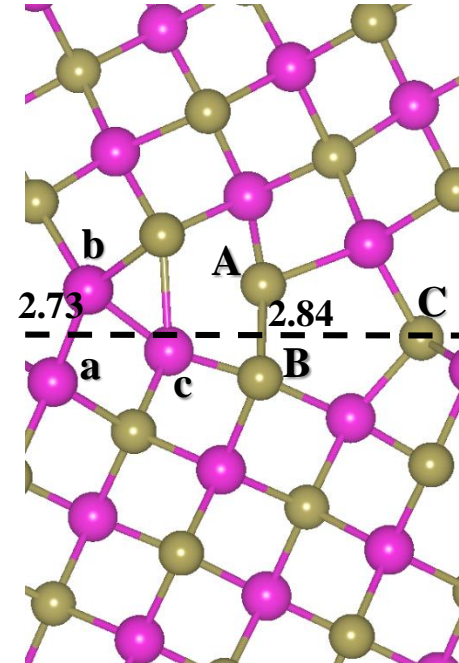
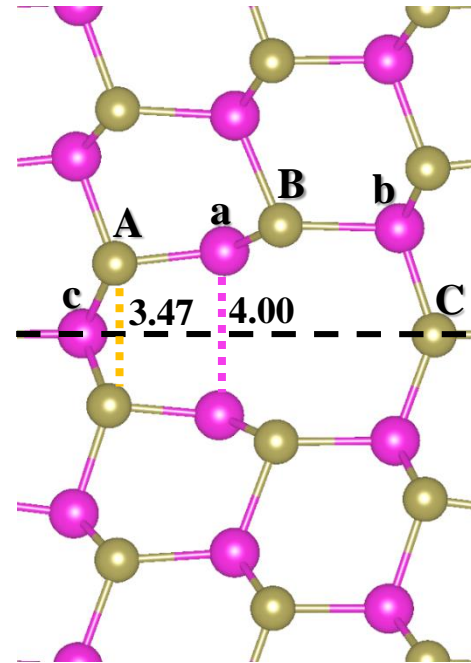
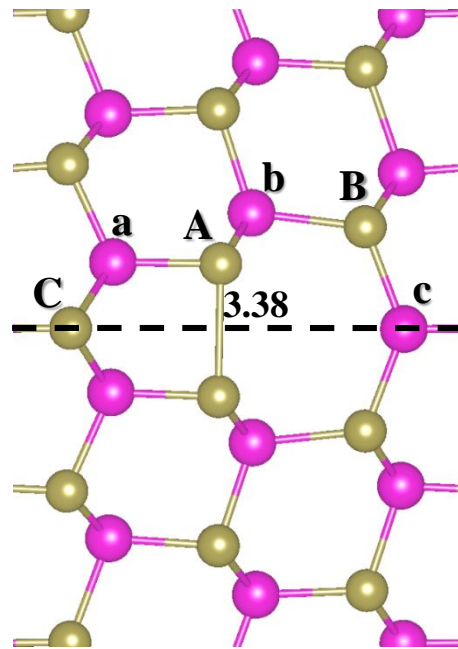
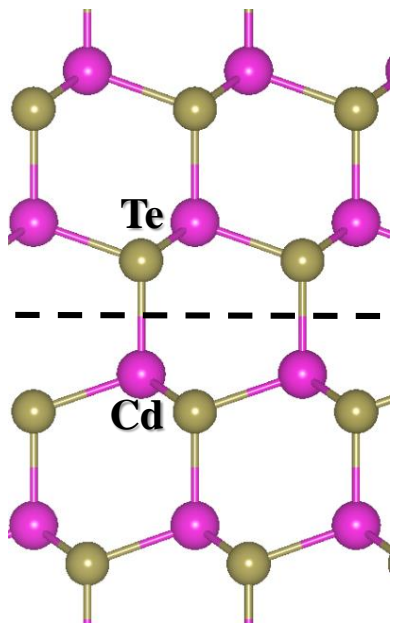
Four Grain Boundaries

$\Sigma 3$ (111)

$\Sigma 3$ (112) Te core

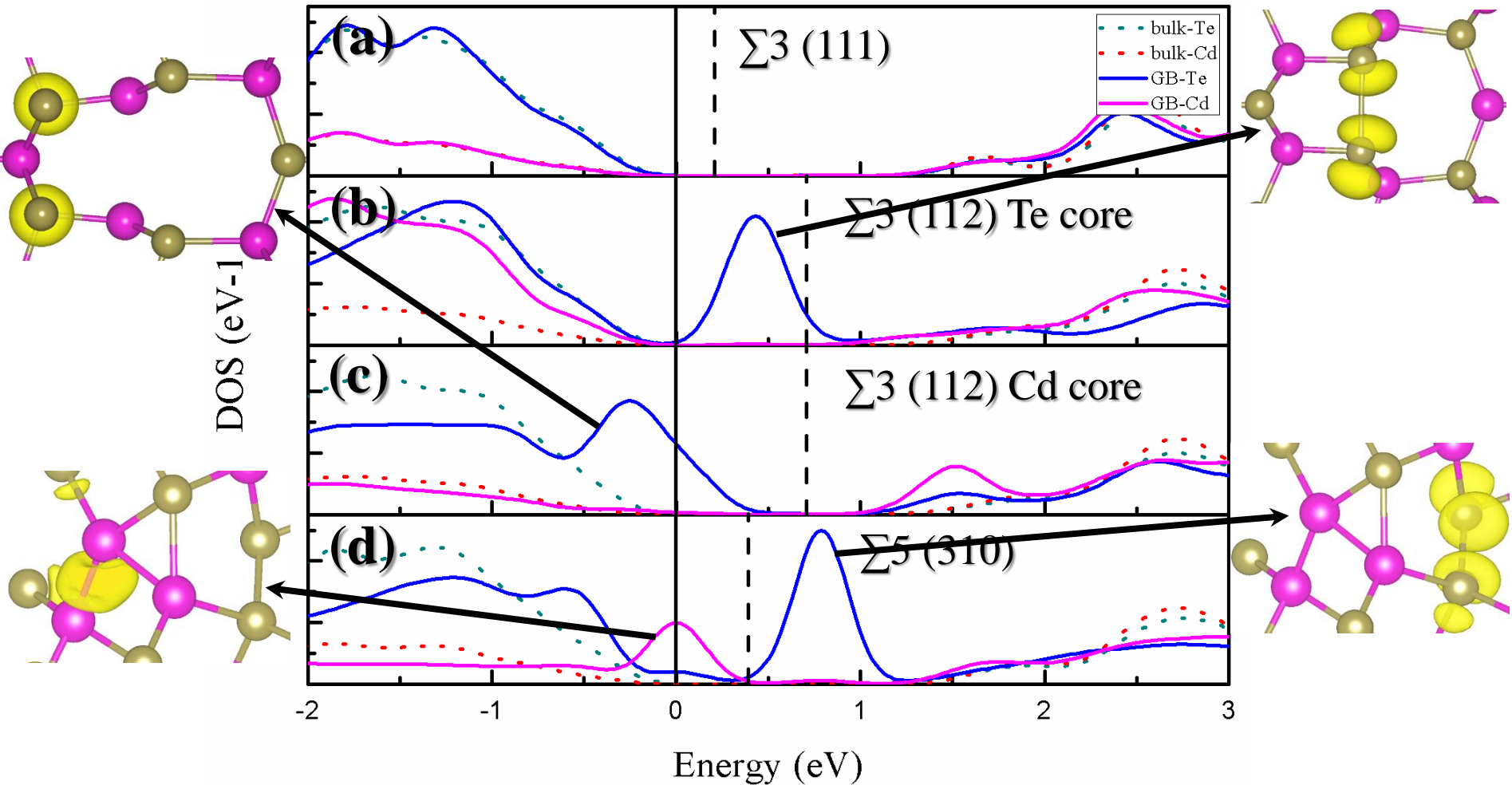
$\Sigma 3$ (112) Cd core

$\Sigma 5$ (310)





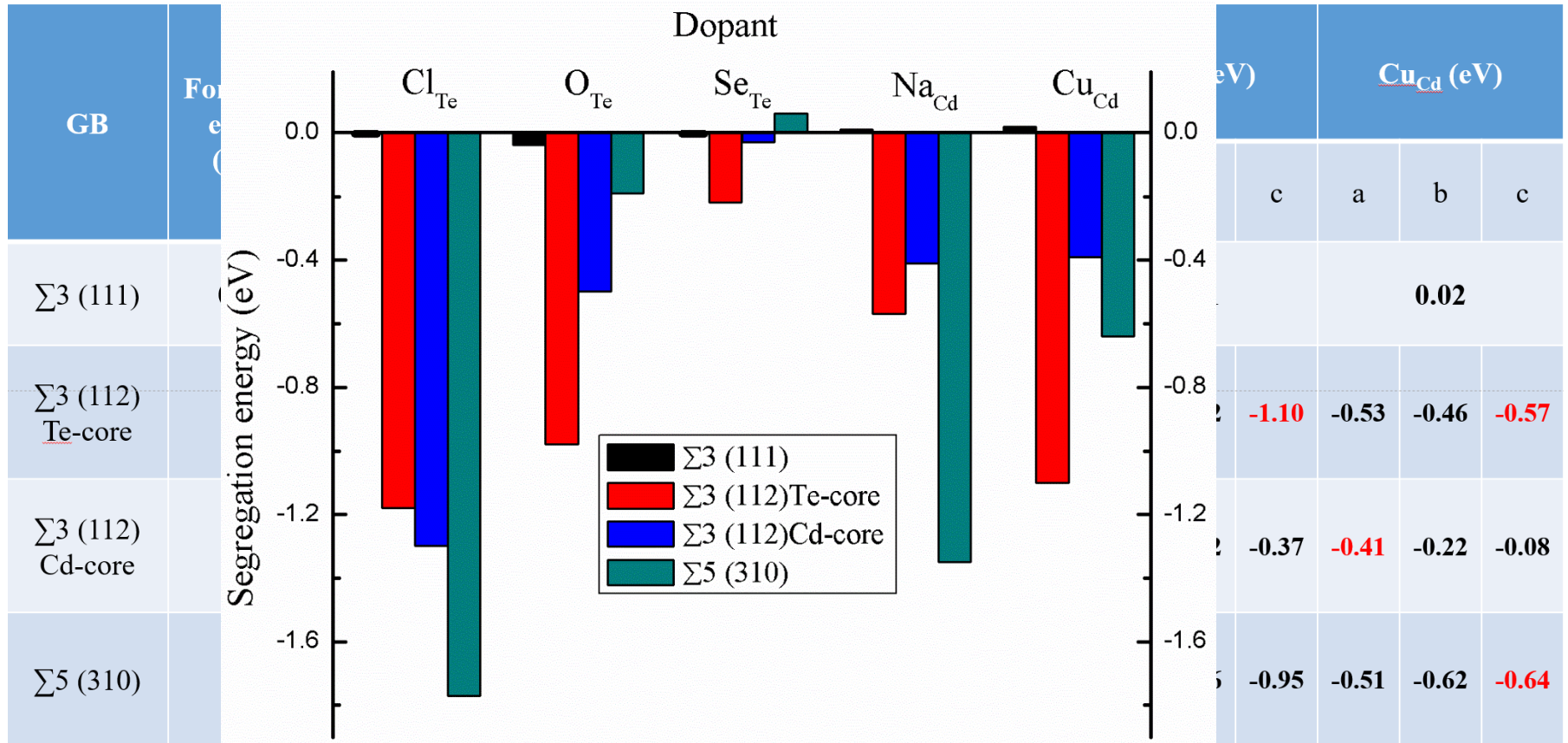
Electric Properties



1. No gap state in $\Sigma 3 (111)$
2. One deep gap state in $\Sigma 3 (112)$ Te core
3. One shallow gap state in $\Sigma 3 (112)$ Cd core
4. One deep and one shallow gap state in $\Sigma 5 (310)$



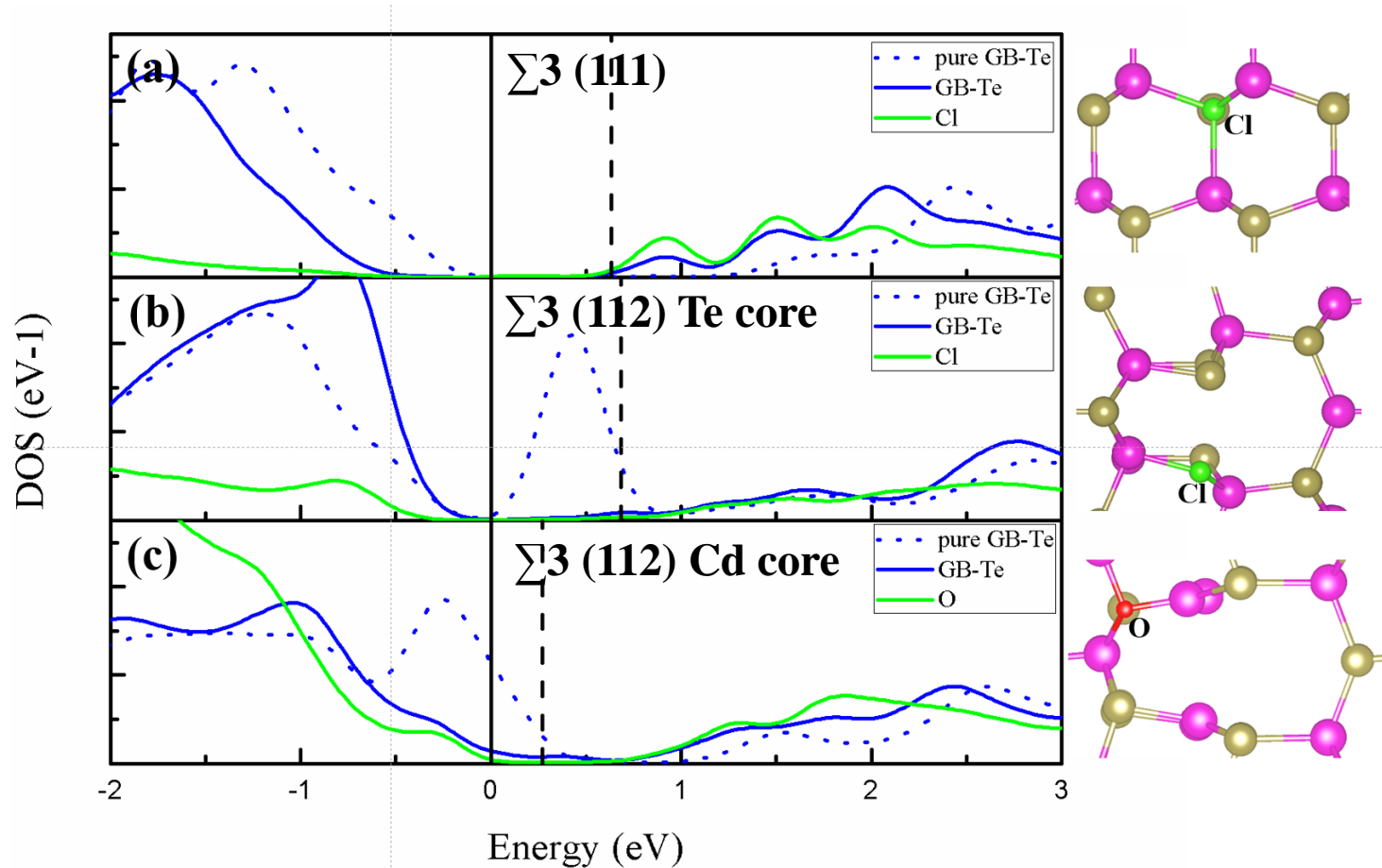
Segregation Energy



1. No segregation behavior in $\Sigma 3$ (111)
2. Almost no segregation behavior in dopant Se
3. All dopants (except for Se) prefer segregating to GB
4. Cl and Na have a strong tendency to break down dangling bonds



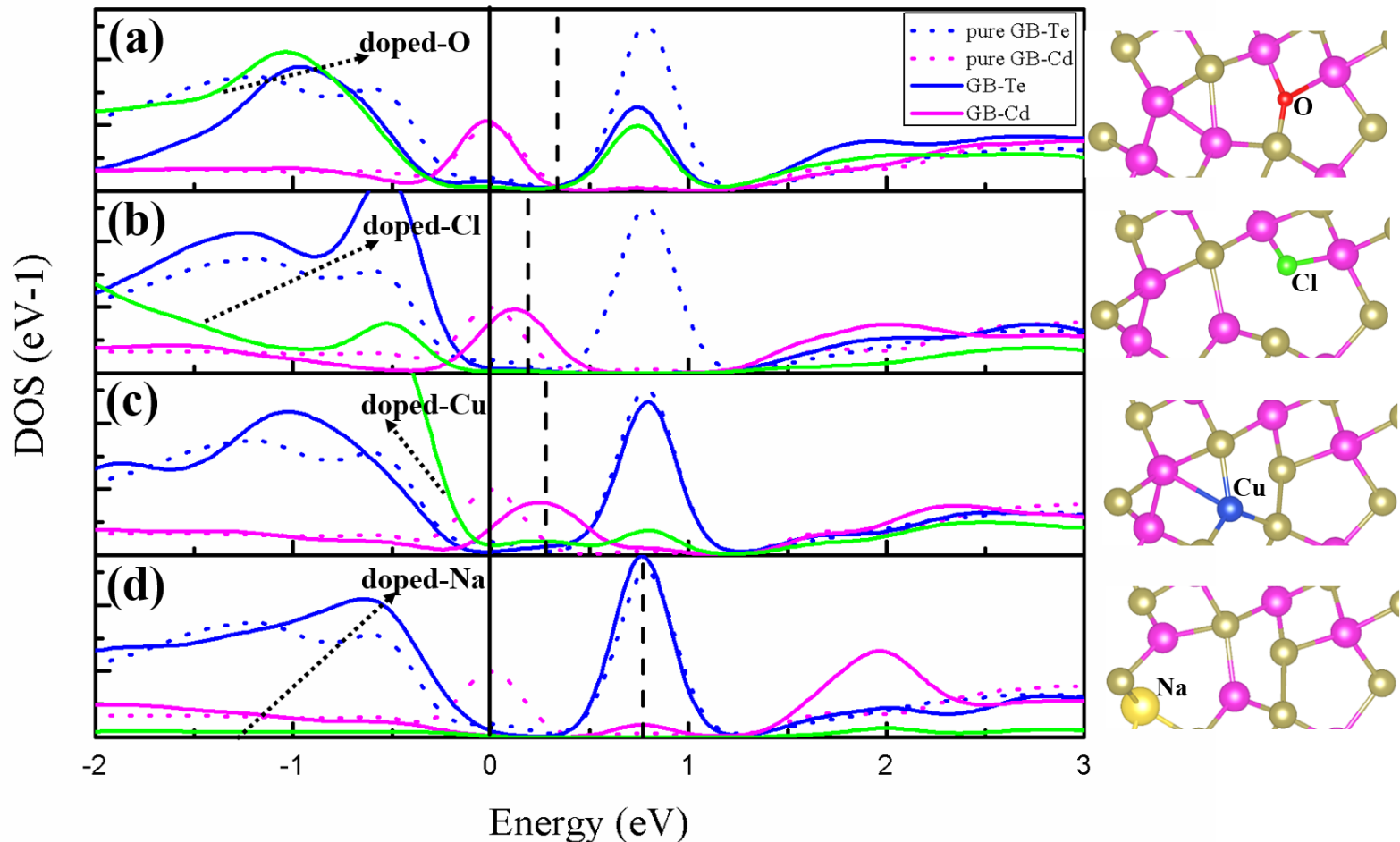
Dopants in $\Sigma 3$



The anion dopants can eliminate gap states by breaking down the dangling bonds.



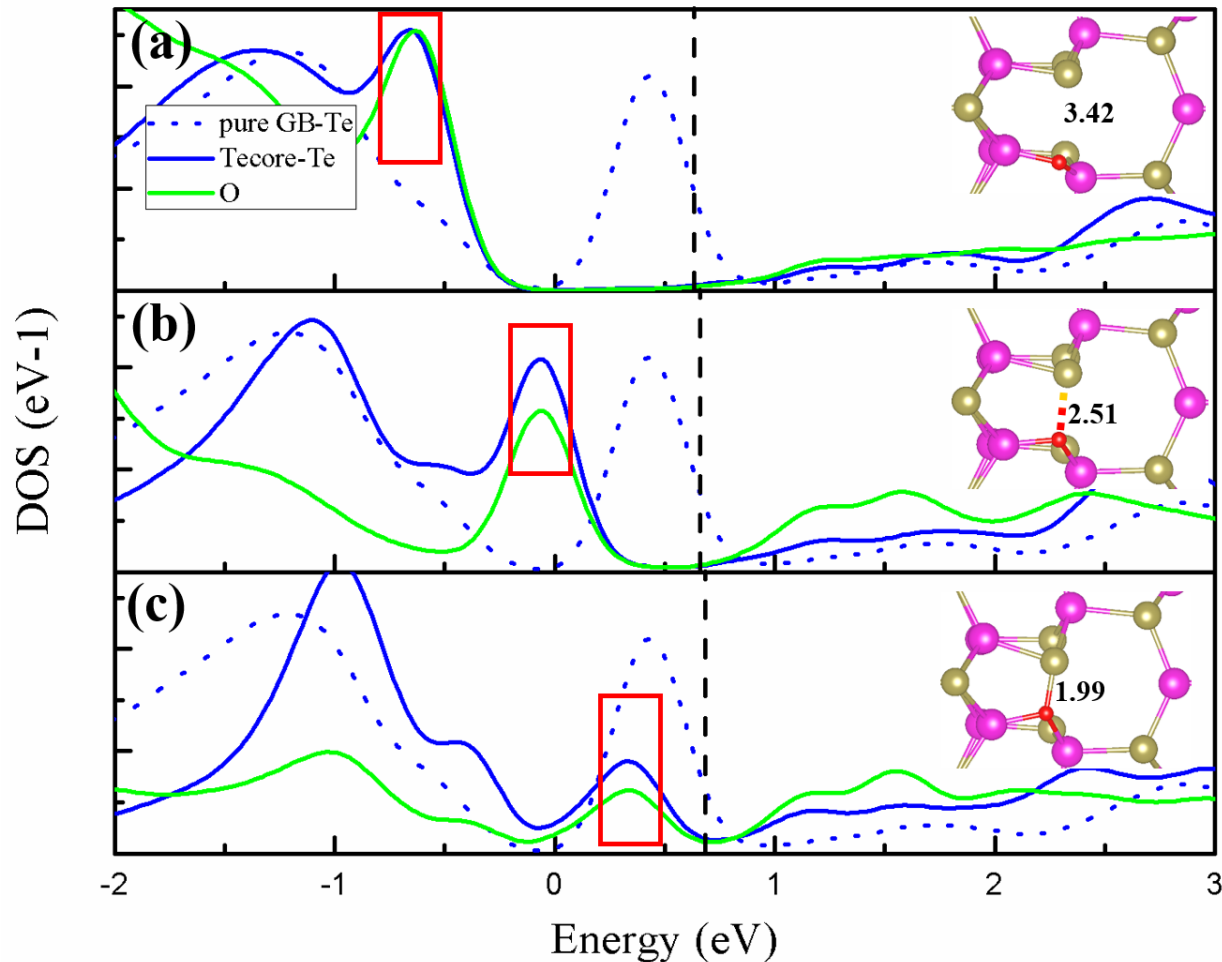
Dopants in $\Sigma 5$



Cl_{Te} can eliminate the deep gap state induced by Te-Te dangling bond, Na_{Cd} can eliminate the shallow gap state induced by Cd-Cd dangling bond

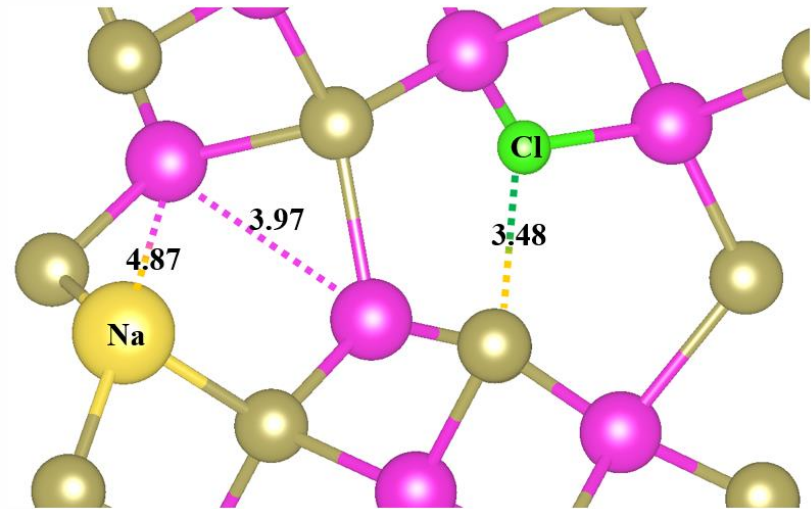
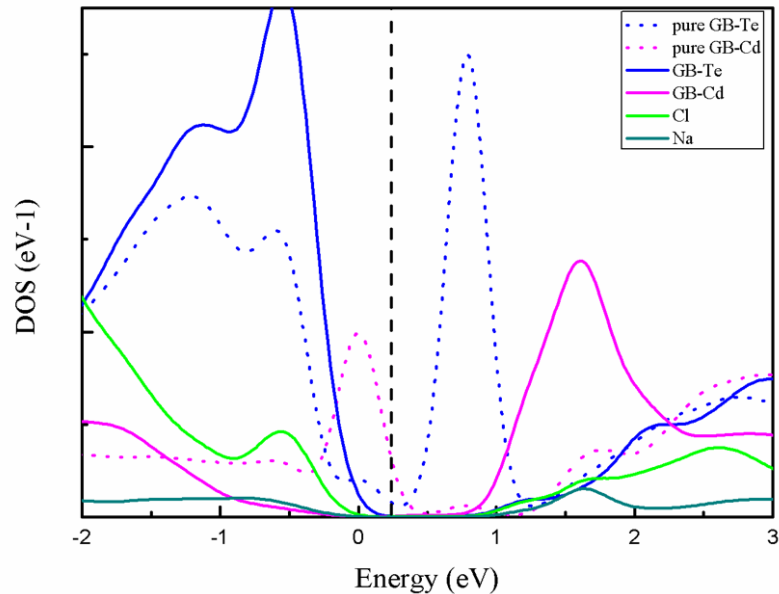


Shift of Gap State



The position of gap state is determined by the dangling bond length of O-Te.

Cl, Na Co-doping in $\Sigma 5$



Cl, Na co-doping can remove all gap states in GB $\Sigma 5$ (310), which is helpful to whole performance.



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Conclusion

- 1. GB $\Sigma 3$ (111) is the most stable and clean one.**
- 2. All extrinsic dopants except for Se prefer segregating to GB.**
- 3. O_{Te} can only passivate the long Te-Te DB, Cl_{Te} can passivate both long and short Te-Te DB, Na_{Cd} can break down Cd-Cd DB.**
- 4. Cl, Na co-doping can effectively passivate all GBs in CdTe.**



Acknowledgement



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