V_{OC} impact of orientation-dependent χ in anisotropic PV absorbers

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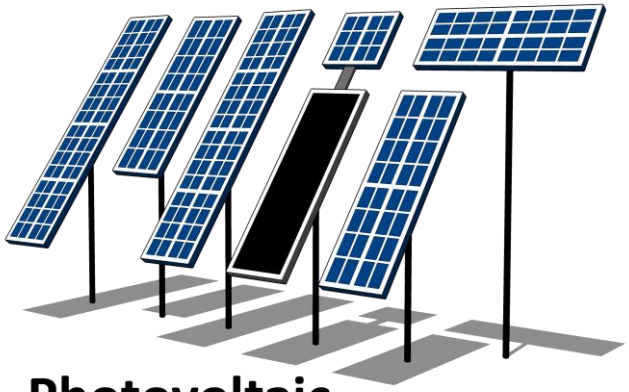

Photovoltaic Research Laboratory

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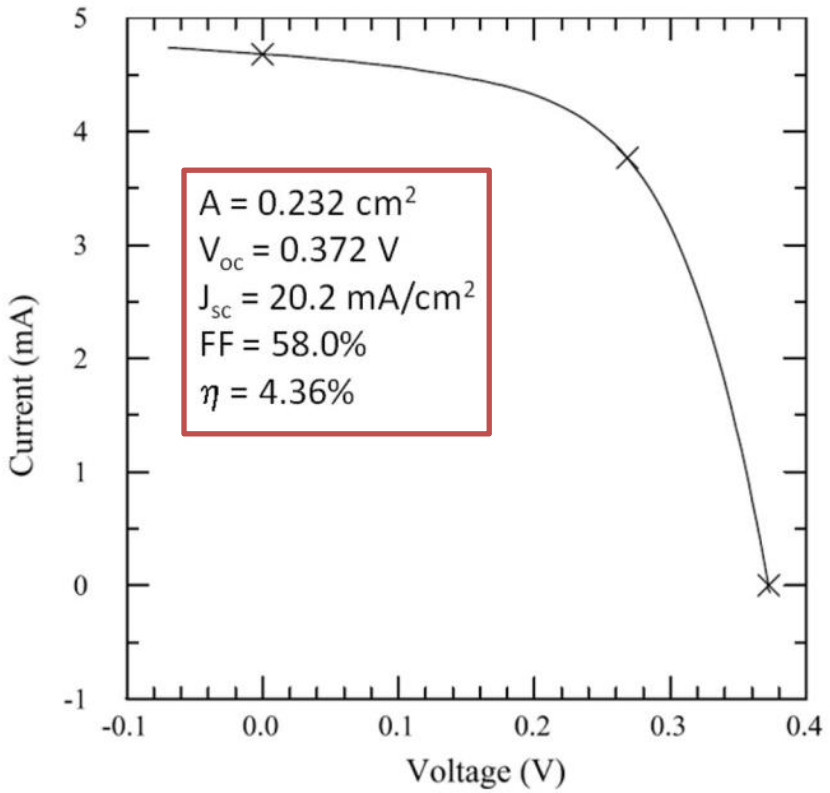
V_{OC} deficit in SnS

- Many PV material systems are plagued by low V_{OC}
- CZTS, WS_2, FeS_2, **SnS**



$$V_{OC}^{deficit} = \frac{E_g}{q} - V_{OC}$$

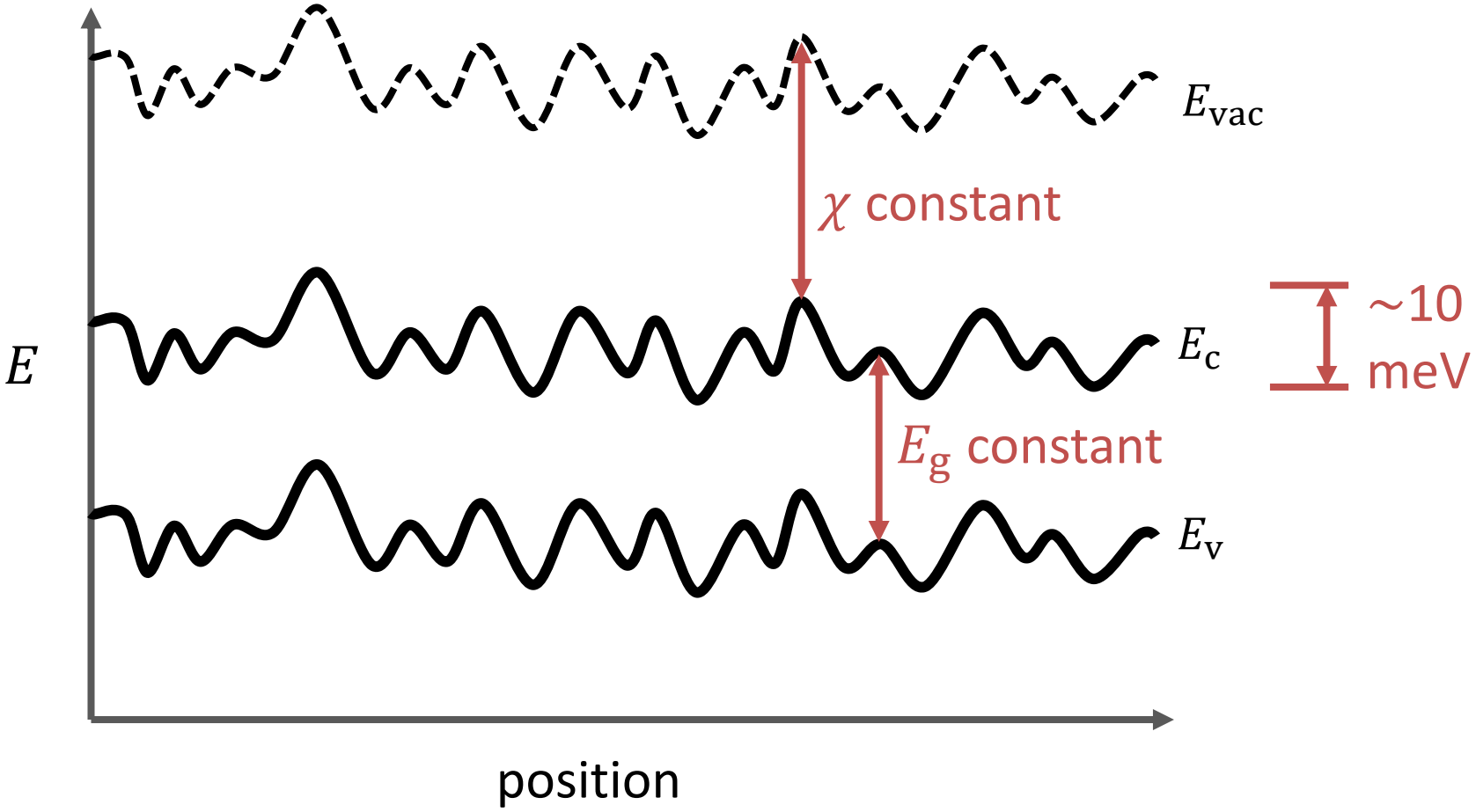
$$= 728 \text{ mV}$$

What causes low V_{OC}?

P. Sinsermsuksakul *et al.*, Adv. Energy Mater. 4, (2014).

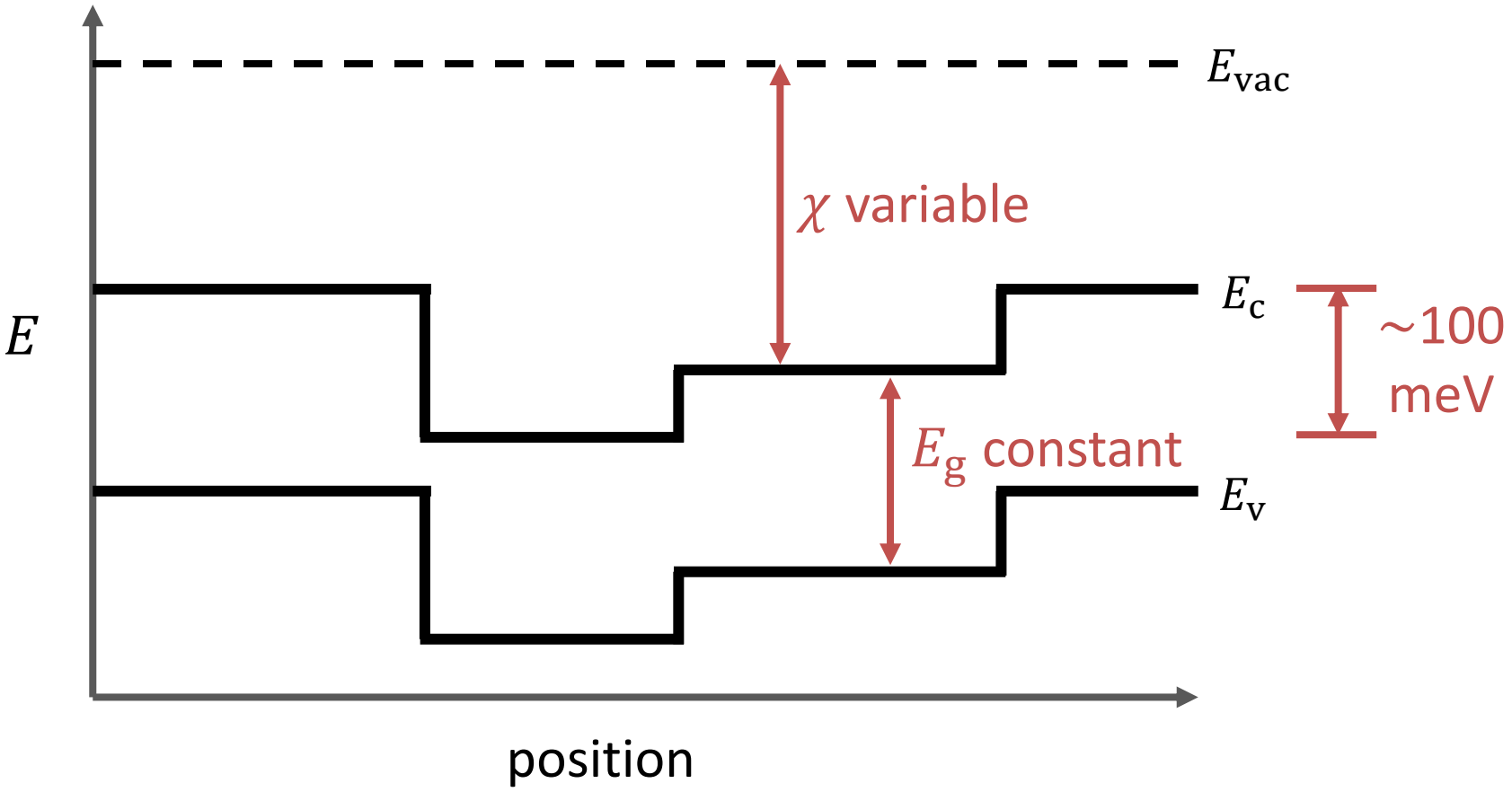
Band fluctuations: constant χ

- $V_{\mathrm{OC}}^{\mathrm{deficit}}$ significantly influenced by electrostatic potential fluctuations[1,2]

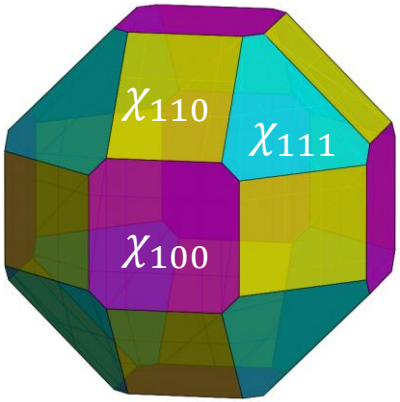


[1,2]J.H. Werner *et al.*, Thin Solid Films 480-481, 399 (2005).
[1,2]Gokmen *et al.*, Applied Physics Letters 103 (2013)

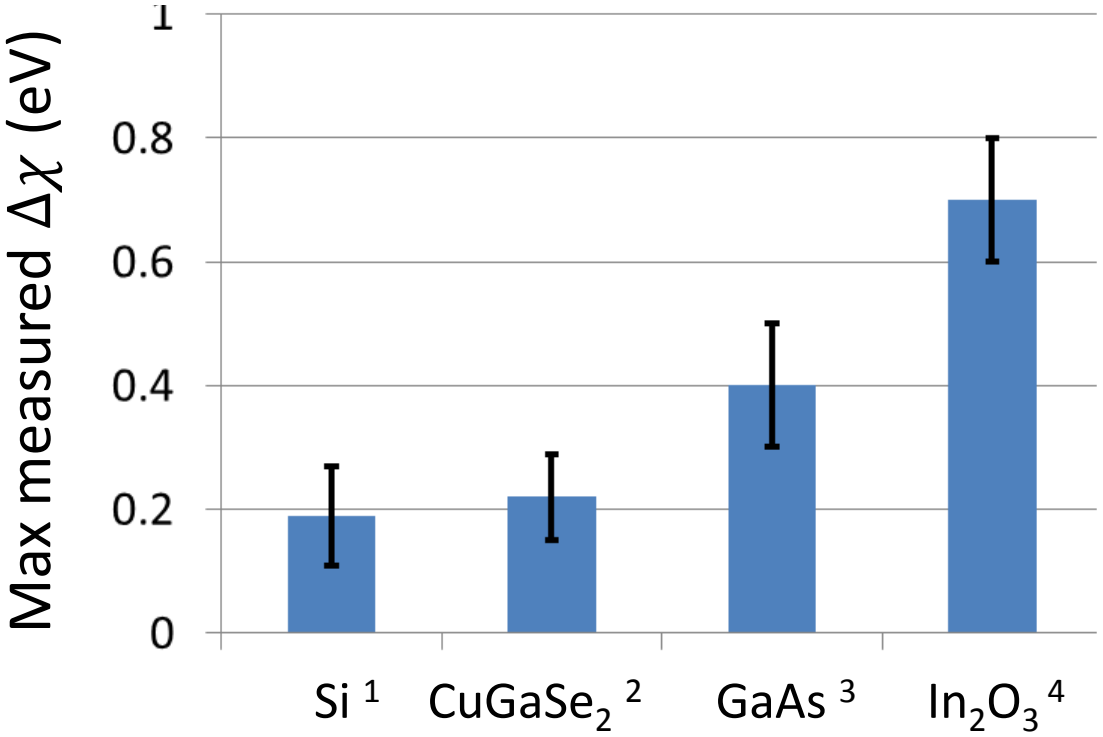
Band fluctuations: variable χ



Surfac n-dependence of electron affinity



$$\Delta\chi = \chi_{hkl} - \chi_{h'k'l'}$$



Wulff construction: Zucker *et al.*, *Journal of Materials Science* 47:8290-8302 (2012).

[1]J.W. Keister *et al., J. Vac. Sci. Technol. B 17, 1831 (1999).*

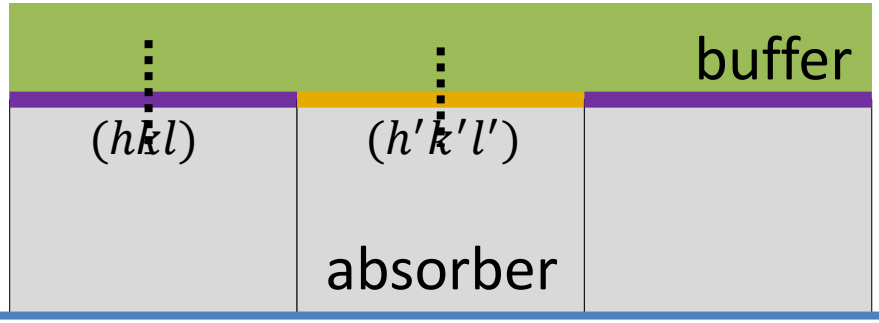
[2]S. Sadewasser *et al., Appl. Phys. Lett. 80, 2979 (2002).*

[3]W. Ranke, *Phys. Rev. B 27, 7807 (1983).*

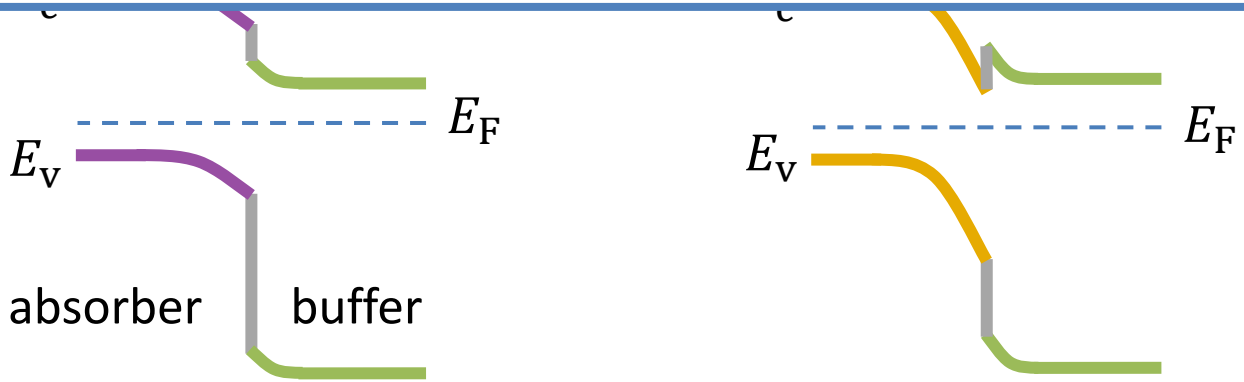
[4]M. Hohmann *et al., J. Phys. Condens. Matter 23, 334203 (2011).*

[5]V. Stevanović *et al., Appl. Phys. Lett. 104, 211603 (2014).*

Lateral CBO variation due to grain orientation



What is the impact of orientation-dependent electron affinity on SnS device performance?



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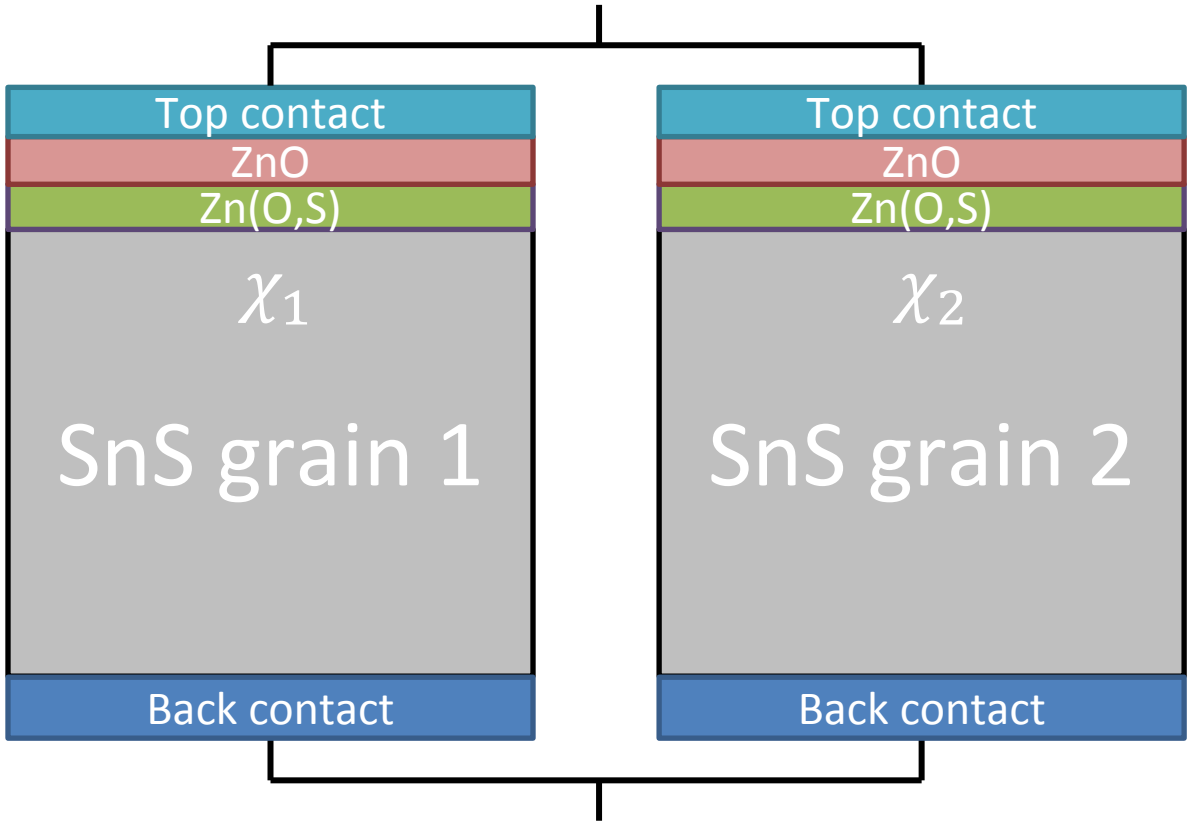
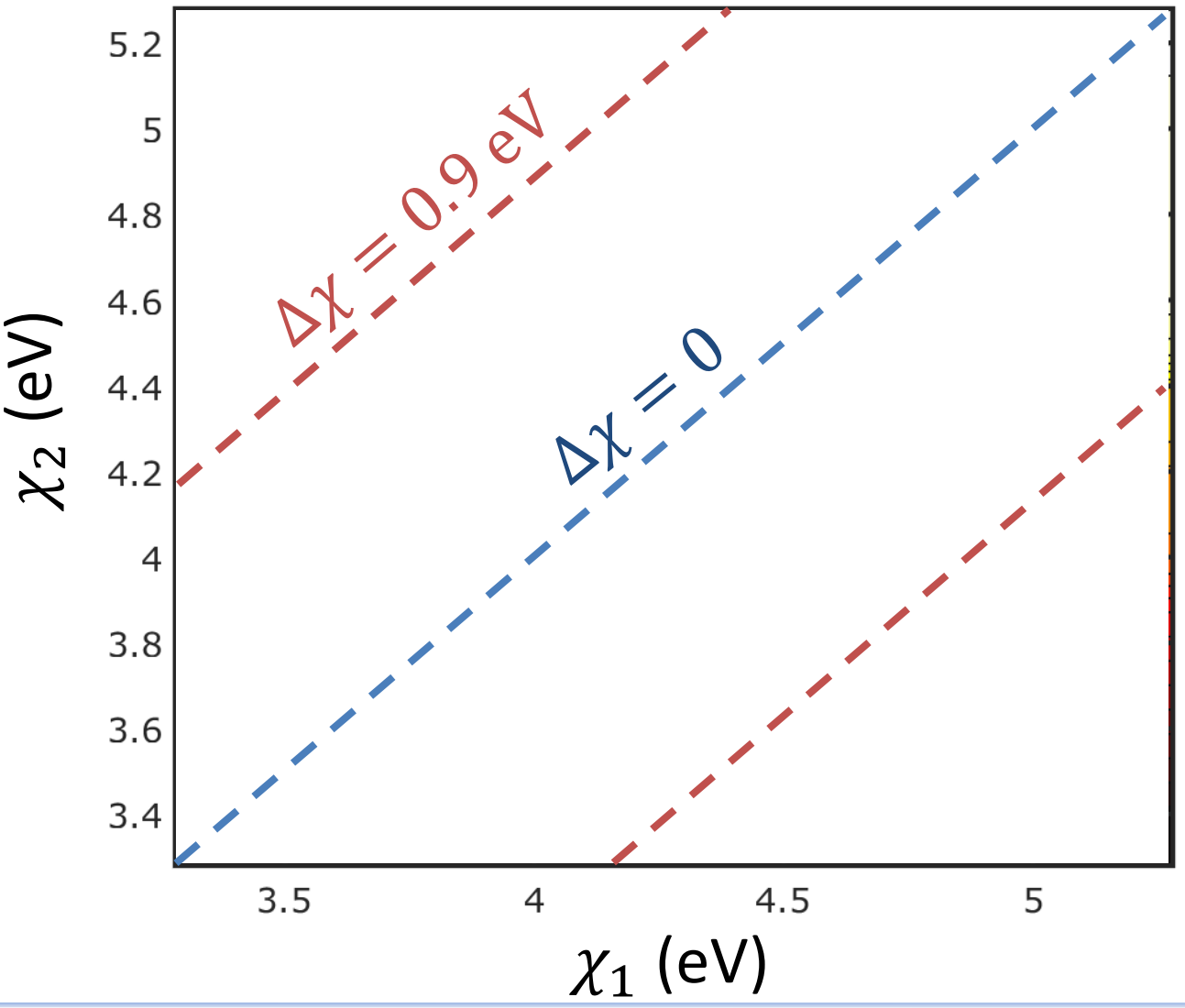
Simple test case: two-grain model



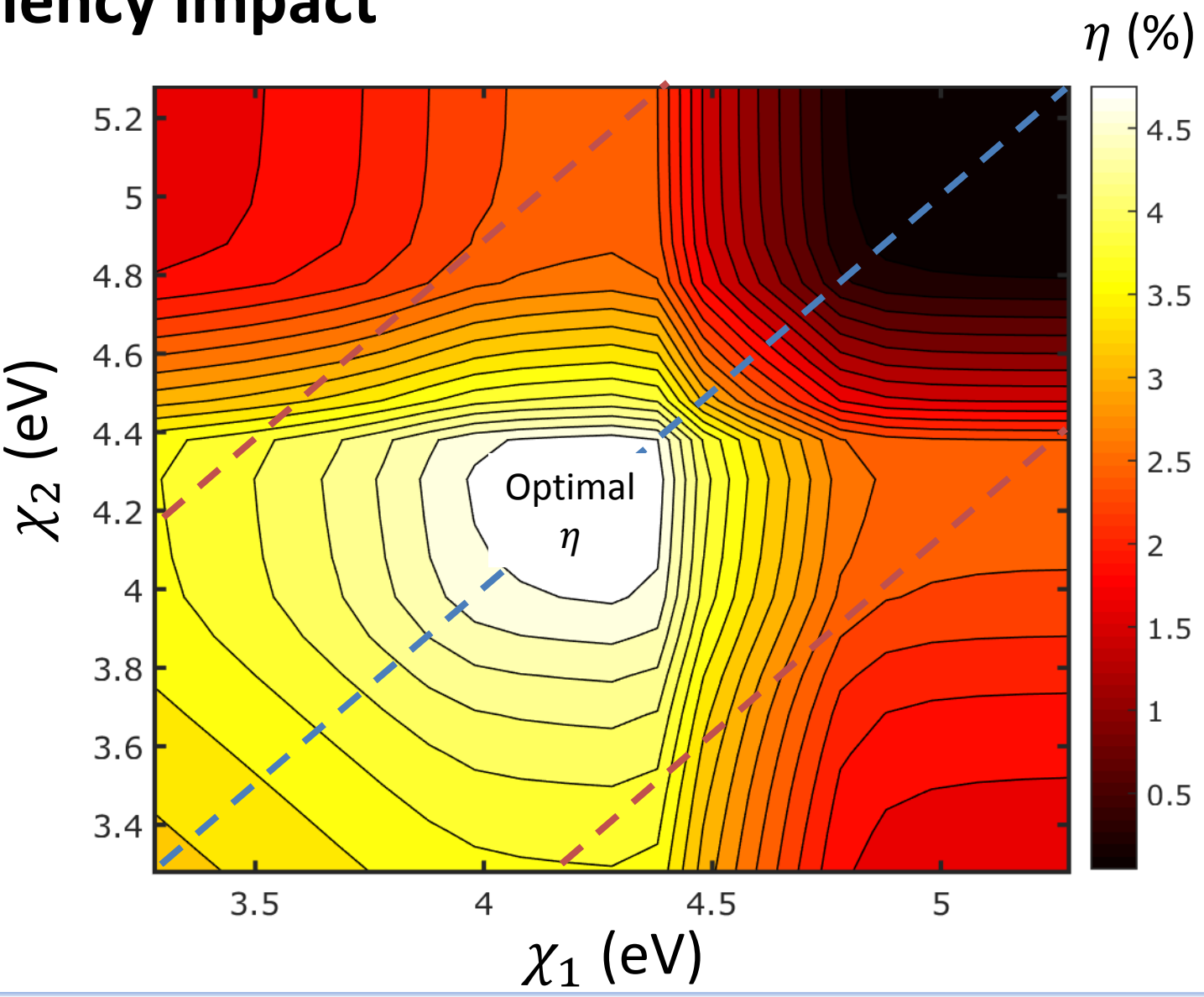
Single stack previously modeled in SCAPS 1D[1]

[1]Mangan *et al.*, J. Appl. Phys. 118, 115102 (2015).

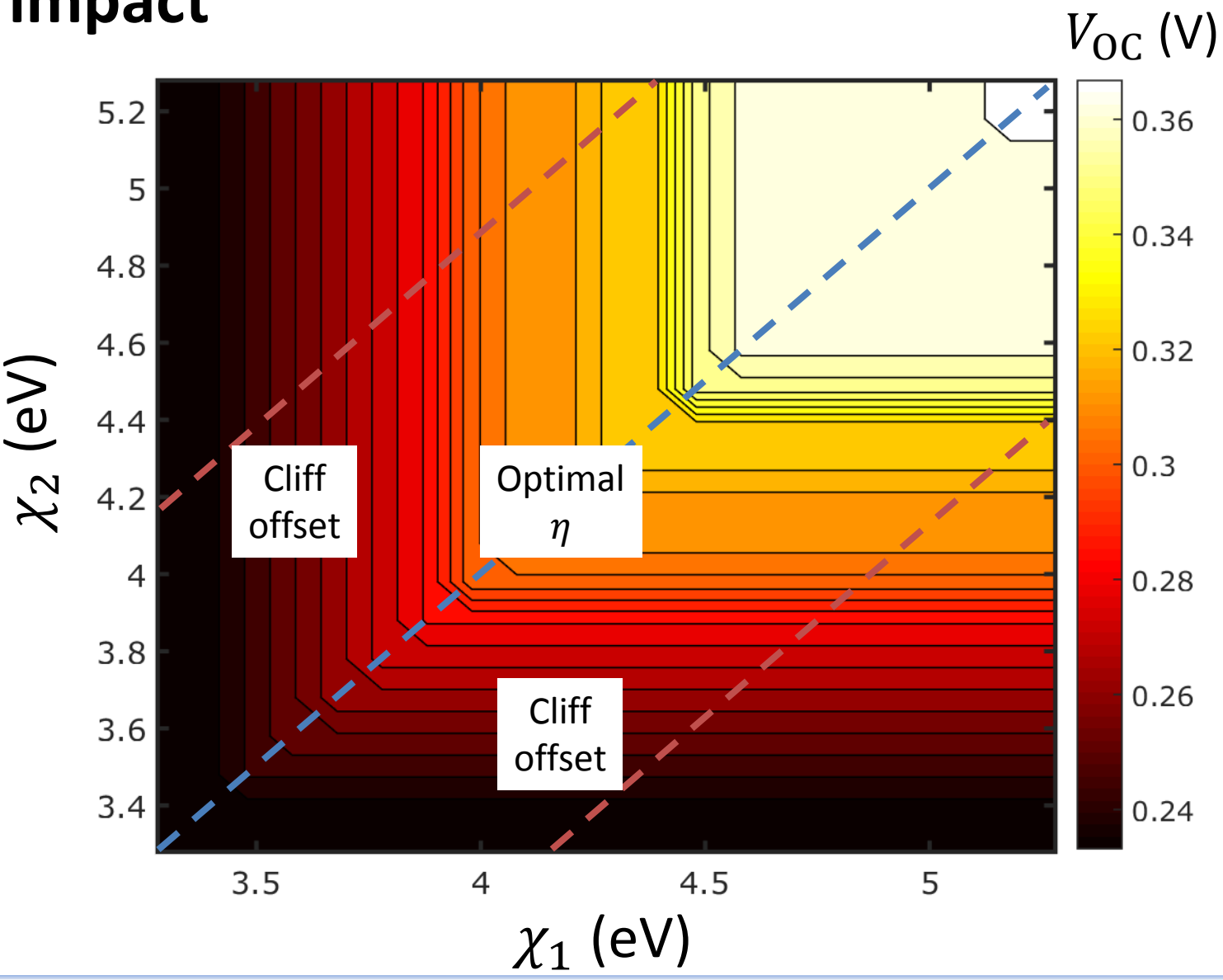
Electron affinity parameter space



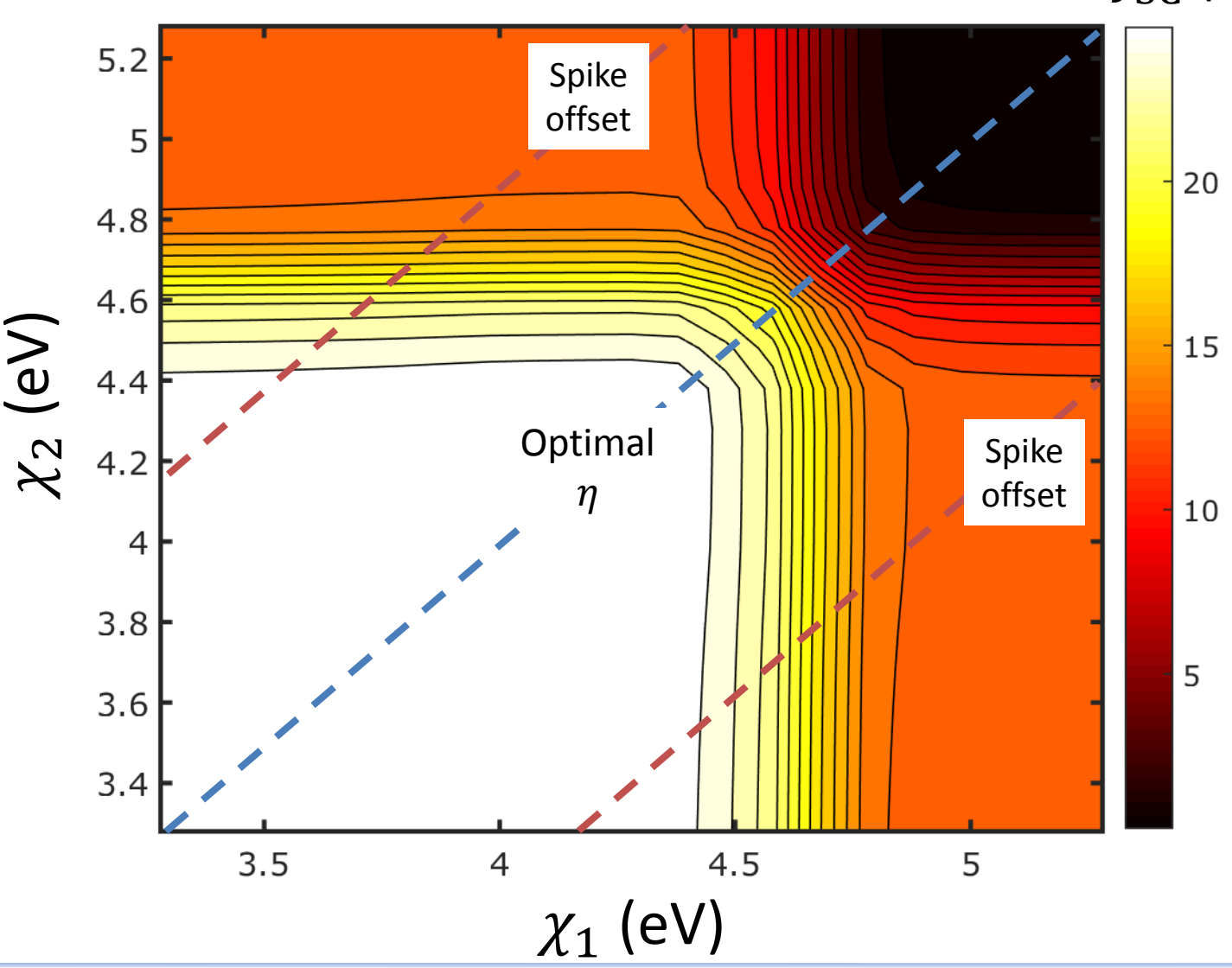
Efficiency impact



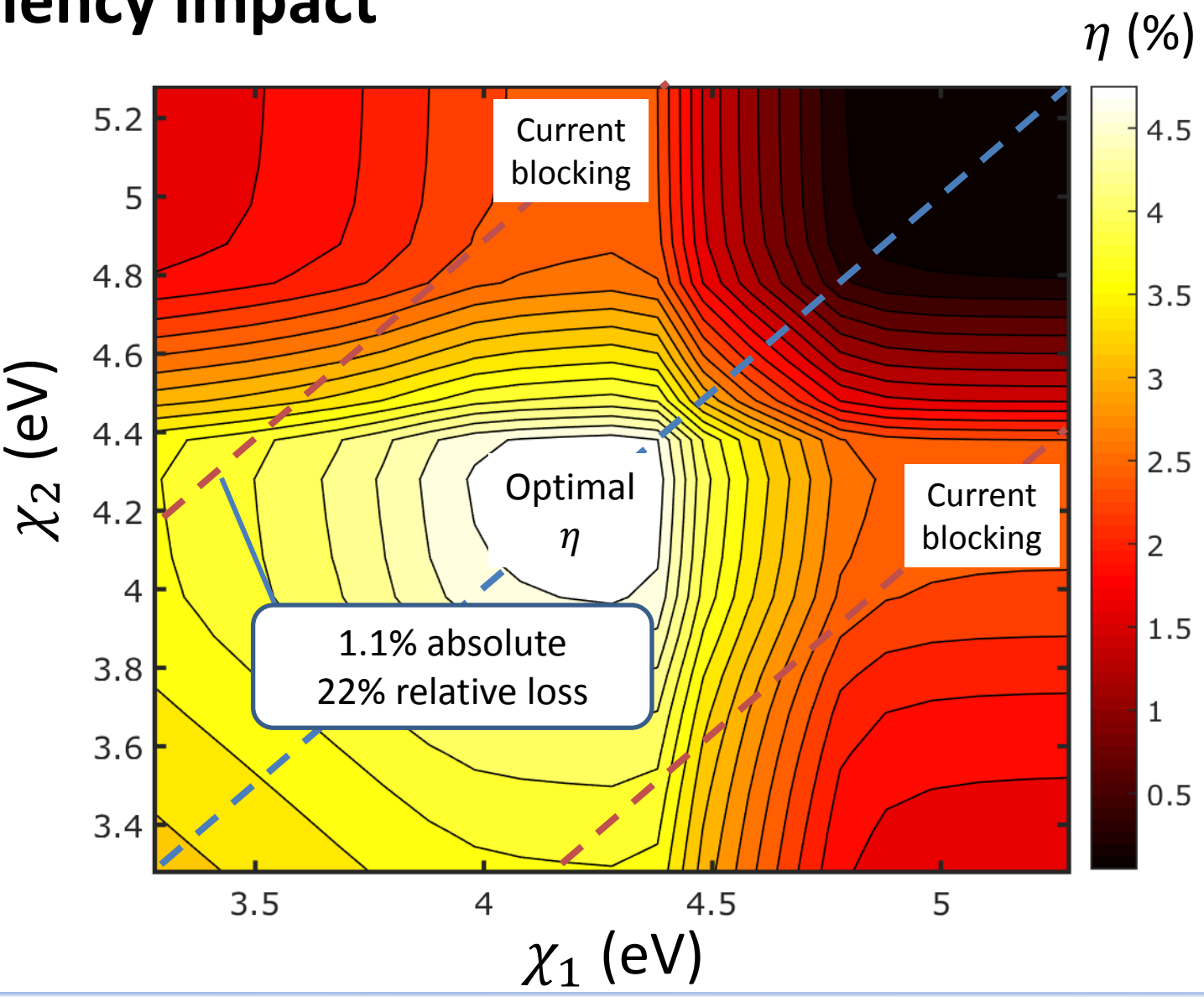
V_{OC} impact


V_{OC} (V)
0.36
0.34
0.32
0.3
0.28
0.26
0.24
χ_2 (eV)
5.2
5
4.8
4.6
4.4
4.2
4
3.8
3.6
3.4
3.5
4
4.5
5
χ_1 (eV)
Cliff offset
Optimal η
Cliff offset

J_{SC} impact


J_{SC} (mA/cm²)
Spike offset
Optimal η
Spike offset
χ_2 (eV)
χ_1 (eV)
5.2
5
4.8
4.6
4.4
4.2
4
3.8
3.6
3.4
3.5
4
4.5
5
20
15
10
5

Efficiency impact

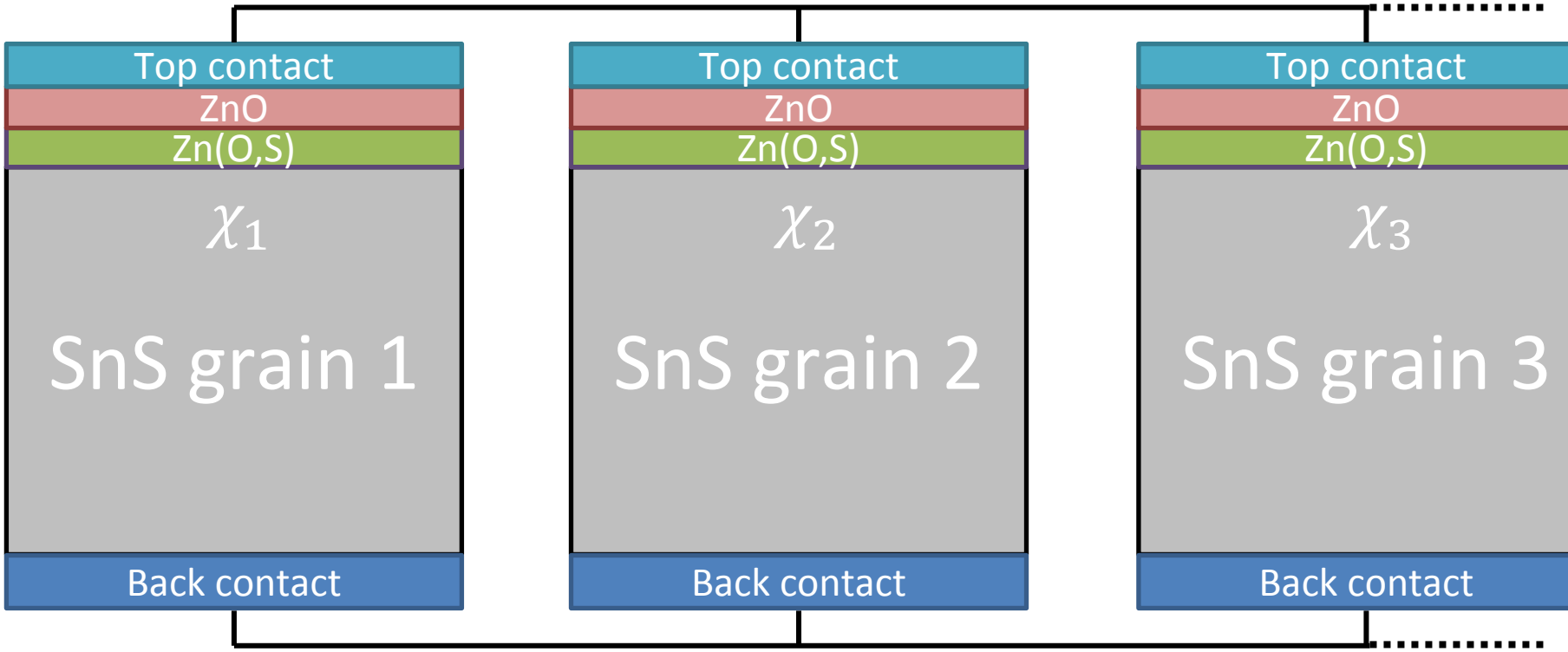


Summary

- Abrupt lateral fluctuations in χ are expected in SnS due to orientation dependence
- Current blocking is worst effect
  - Avoided by optimizing buffer layer
  - V_{OC} still reduced because of cliff offset
  - 22% relative loss in efficiency for $\Delta\chi = 0.9$ eV

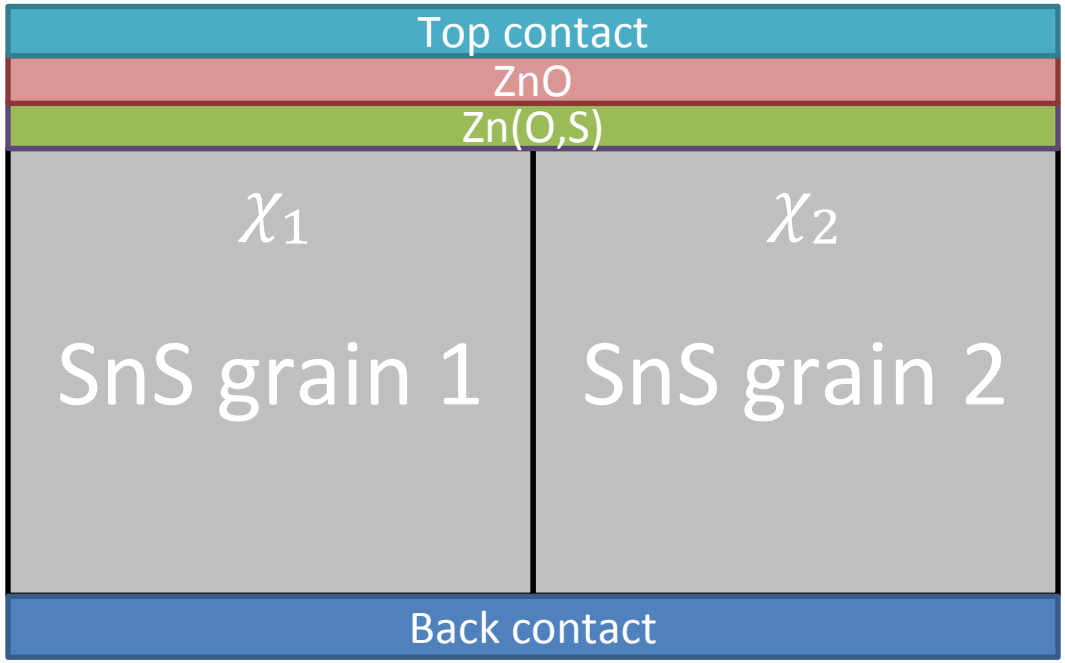
Further work

- Confirm $\chi(hkl)$ in SnS experimentally
- >2 grains in parallel



Further work

- Confirm $\chi(hkl)$ in SnS experimentally
- >2 grains in parallel
- Simulation accounting for 2D carrier flow



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Harvard University
Center for Nanoscale Systems

CMSE
MIT Center for Materials Science and Engineering

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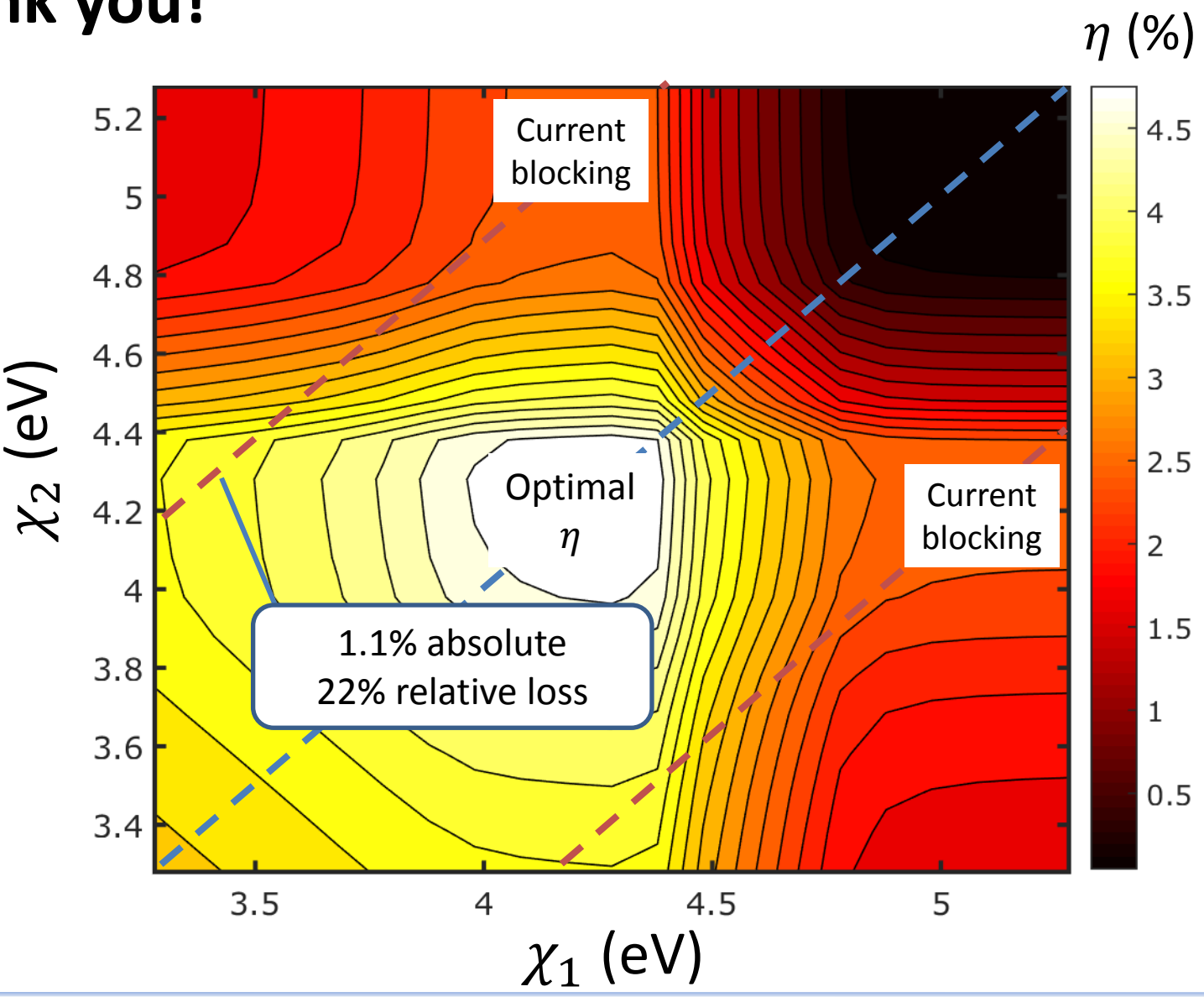
Thank you!


η (%)
Current blocking
Optimal η
Current blocking
1.1% absolute
22% relative loss
χ2 (eV)
χ1 (eV)
5.2
5
4.8
4.6
4.4
4.2
4
3.8
3.6
3.4
3.5
4
4.5
5
4.5
4
3.5
3
2.5
2
1.5
1
0.5