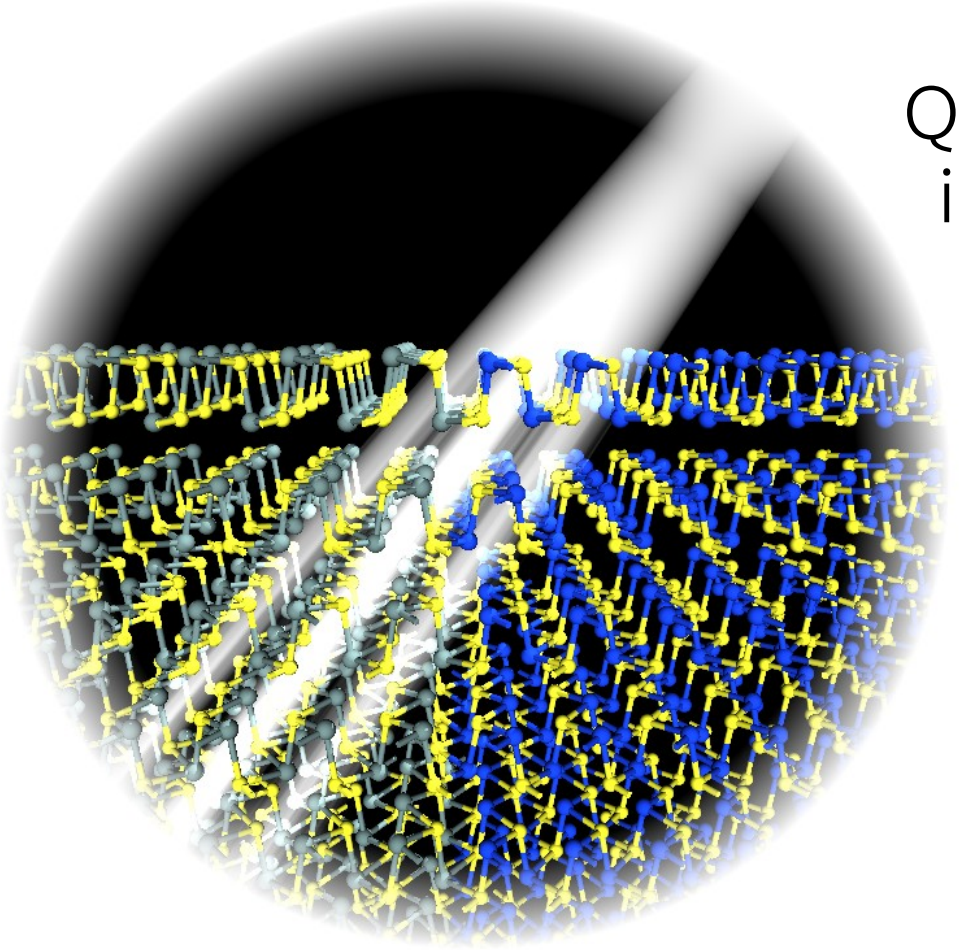

Quasiparticle band structures and interface physics of SnS and GeS

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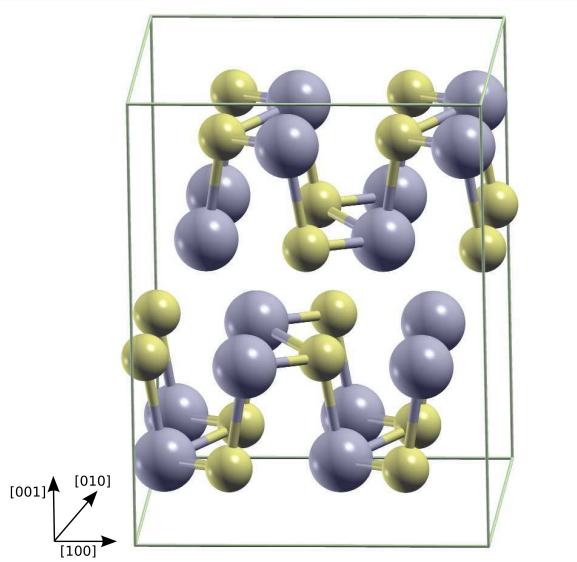
3/21/13

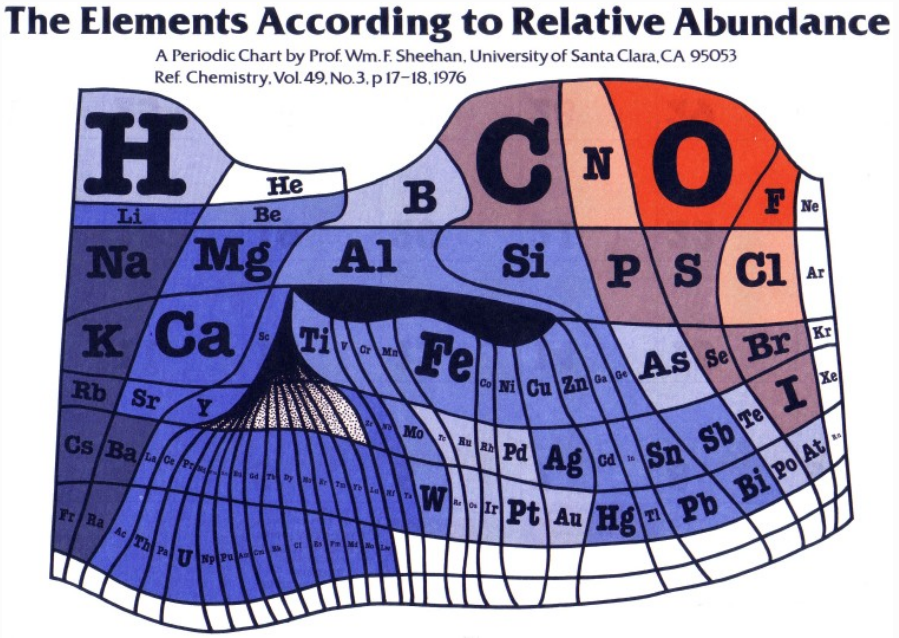
Urgent need for carbon-free energy sources

- efficient?
- low-cost?
- earth abundant?
- nontoxic?

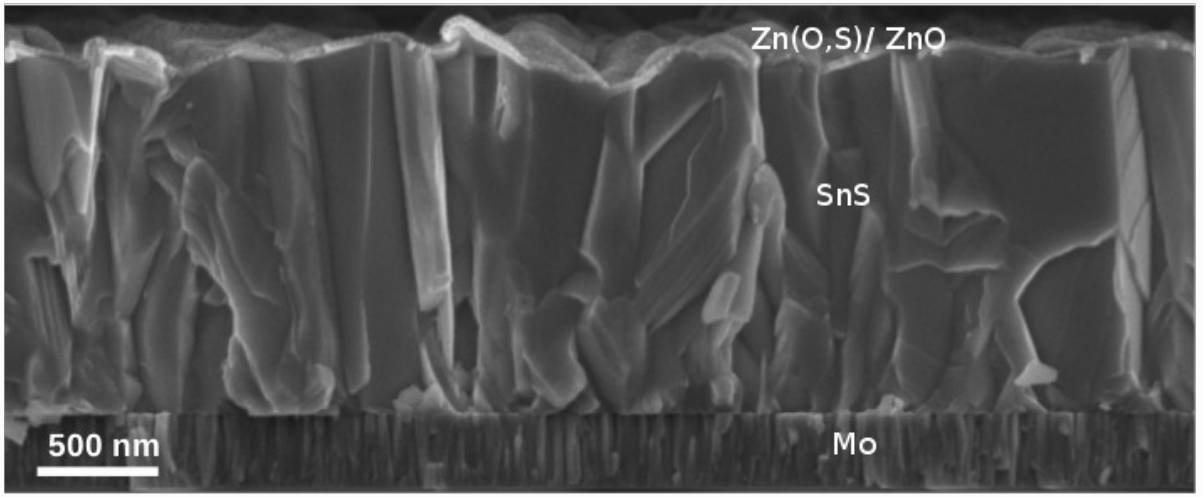
SnS shows promise:

- high absorption ($\alpha > 10^4\,cm^{-1}$)
- suitable band gap (~1.1 – 1.5 eV)
- low-toxicity
- earth–abundant





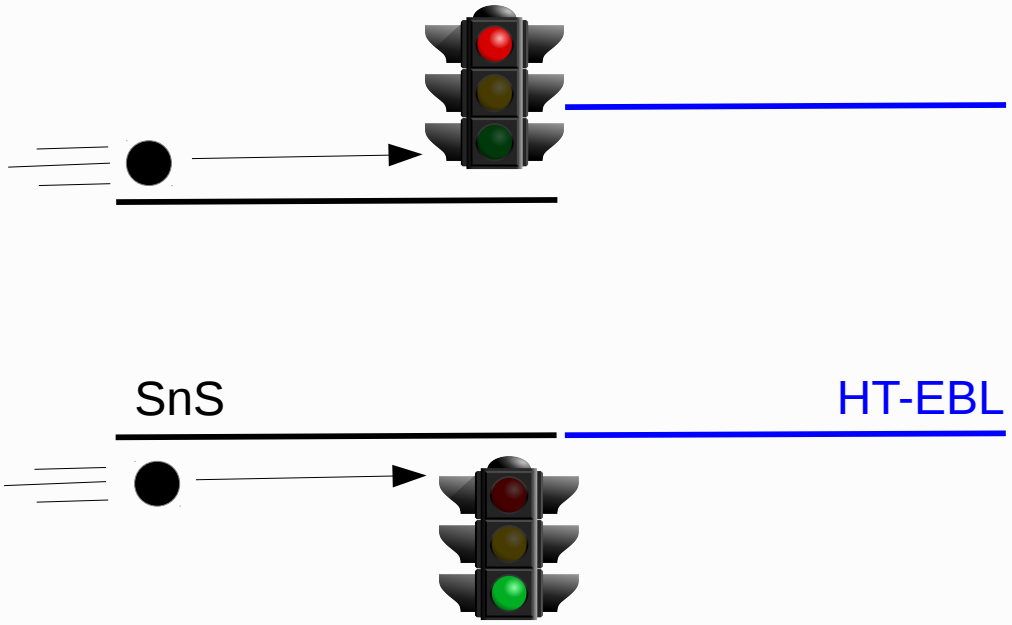
Efficiencies increasing - current record at ~2.5%



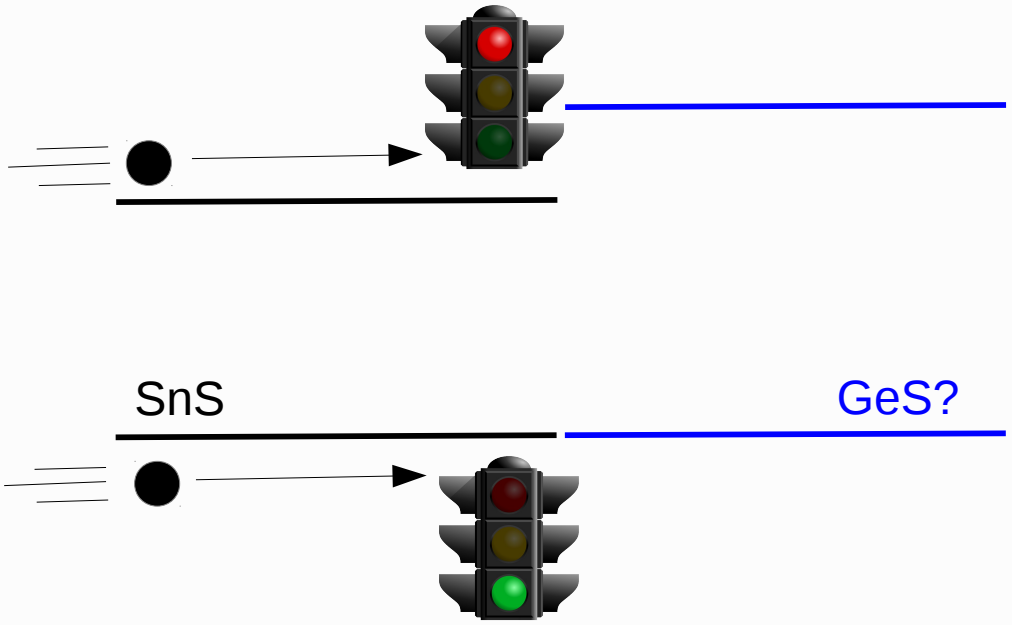
P. Sinsermsukakul, et al., Appl. Phys. Lett. **102**, 053901 (2013)

How much can this be improved?

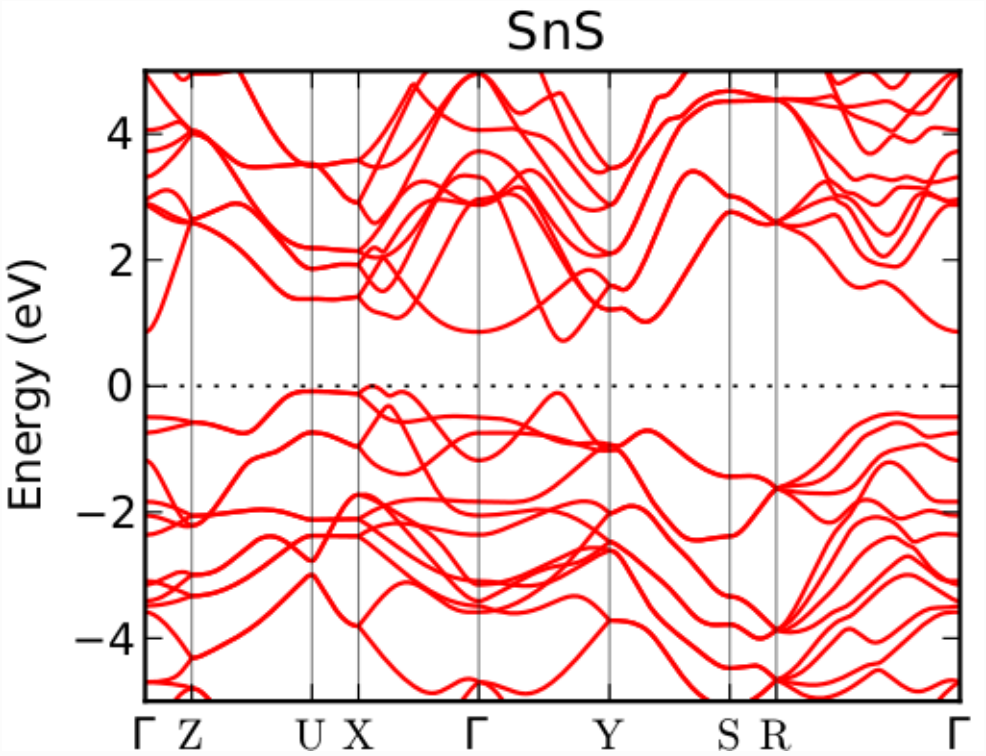
Introduction of a suitable hole-transport electron-blocking layer (HT-EBL)



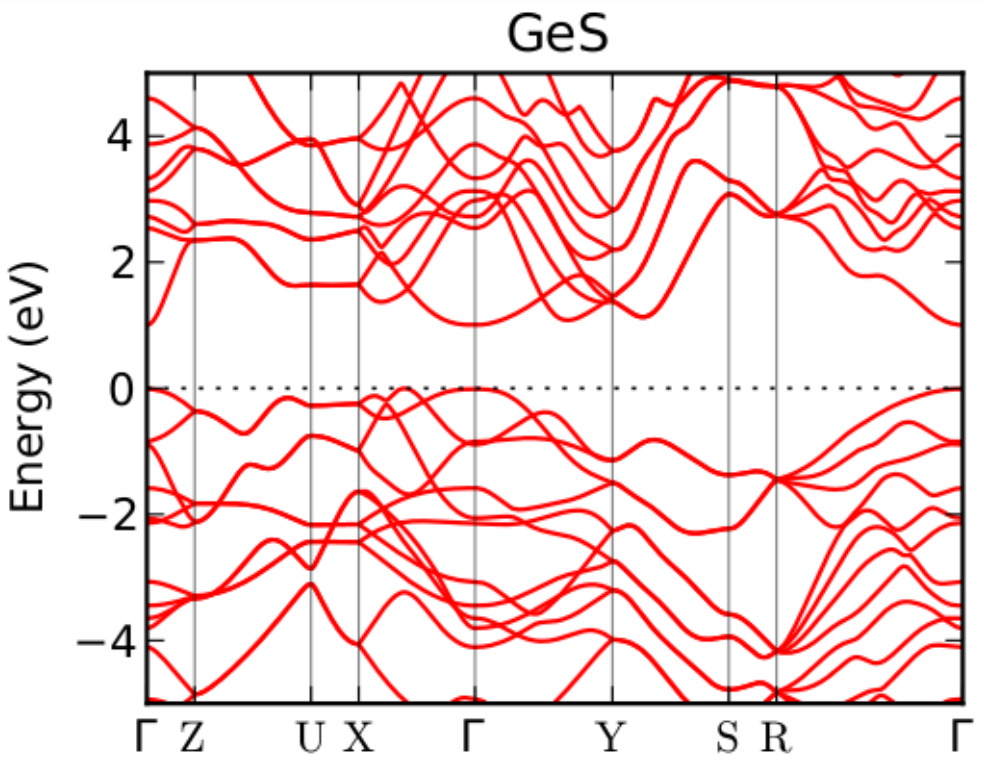
Introduction of a suitable hole-transport electron-blocking layer (HT-EBL)



DFT-LDA planewave pseudopotential results
(experimental lattice parameters)



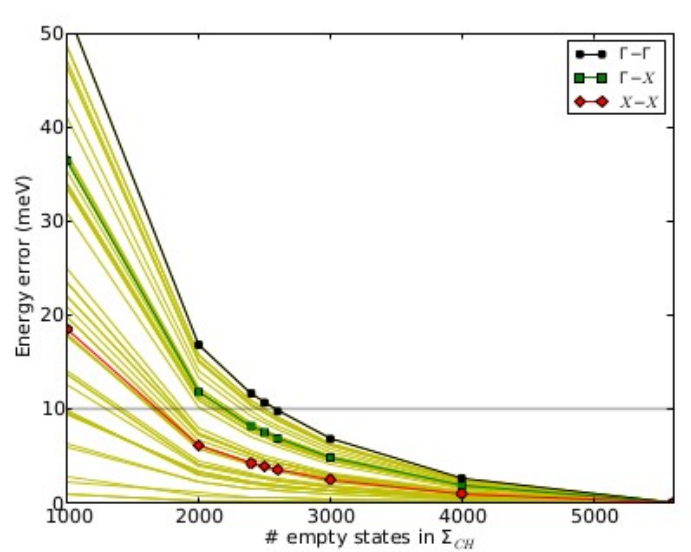
0.72 eV indirect gap

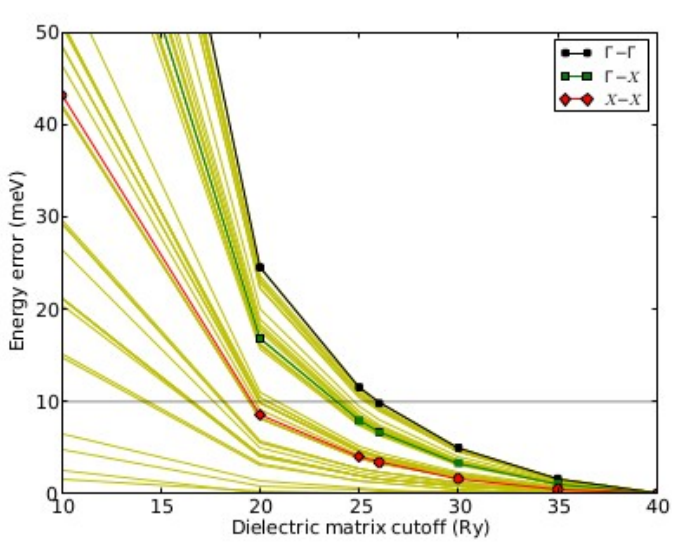


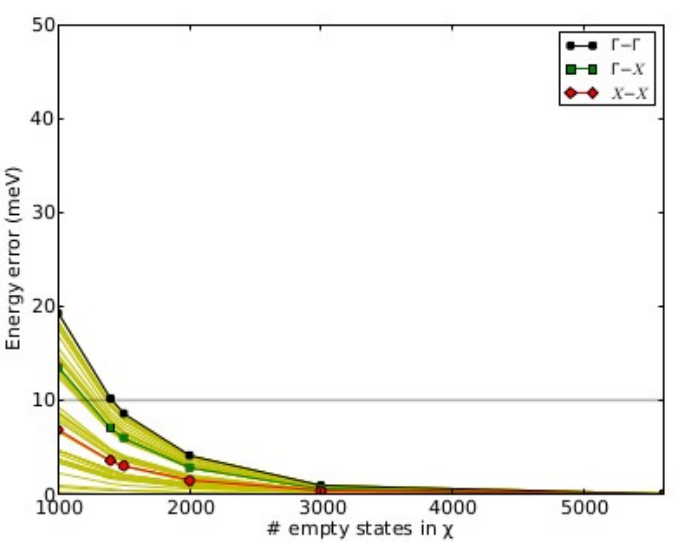
1 eV indirect gap

Quasiparticle energies obtained from GW

Careful attention paid to convergence







SnS: 2600 (1500) states in self-energy (polarizability); 26 Ry cutoff in G-vectors
GeS: 2100 (1000) "" ; 24 Ry ""

5x6x2 BZ samplings used in both

SnS

	T(K)	$E_g^{(T)}$(eV)	E_g^0 (eV)
Theory			
Present work			1.28
Ref. [1] (GW)			1.07
Ref. [2] (GW)			1.07
Experiment			
Ref. [3]	298	1.07	1.20
Ref. [4]	100	1.18	1.22
Ref. [5]	473	1.16	1.37
Ref. [6]	298	1.18	1.31
Ref. [7]	295	1.05	1.16
Ref. [8]	4	1.5	1.5

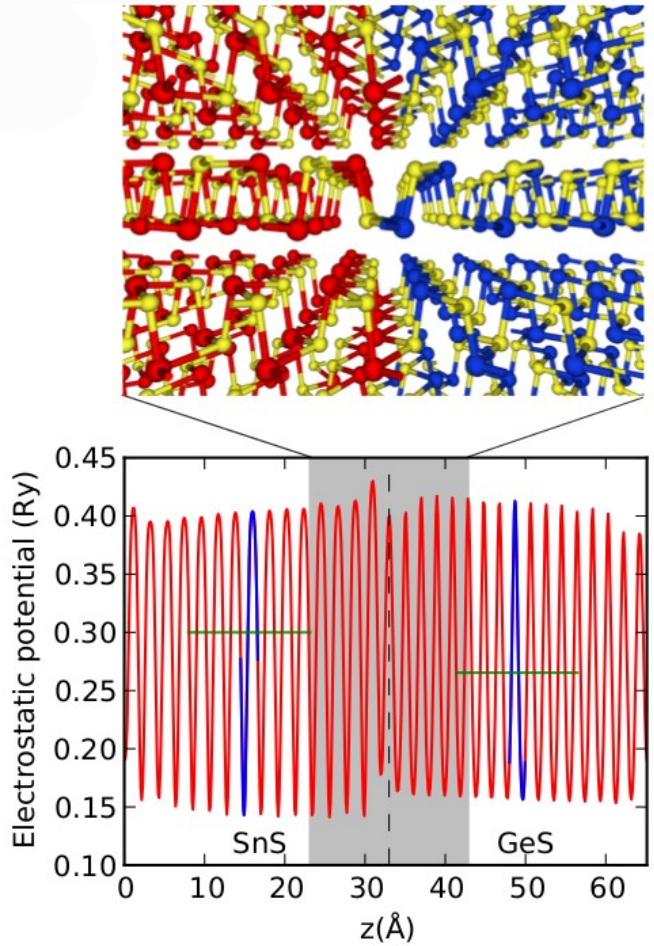
Ref. [1]: Appl. Phys. Lett., **100**, 023104 (2012)
Ref. [2]: Comp. Mater. Sci., **50**, 2872 (2011)
Ref. [3]: J. Phys. Chem. Solids, **15**, 306 (1960)
Ref. [4]: J. Phys. Chem Solids, **35**, 537 (1974)
Ref. [5]: Semicond. Sci. Technol., **11**, 243 (1996)
Ref. [6]: Thin Solid Films, **519**, 7421 (2011)
Ref. [7]: Phys. Rev. B, **41**, 5227 (1990)
Ref. [8]: J. Appl. Phys., **101**, 093522 (2007)

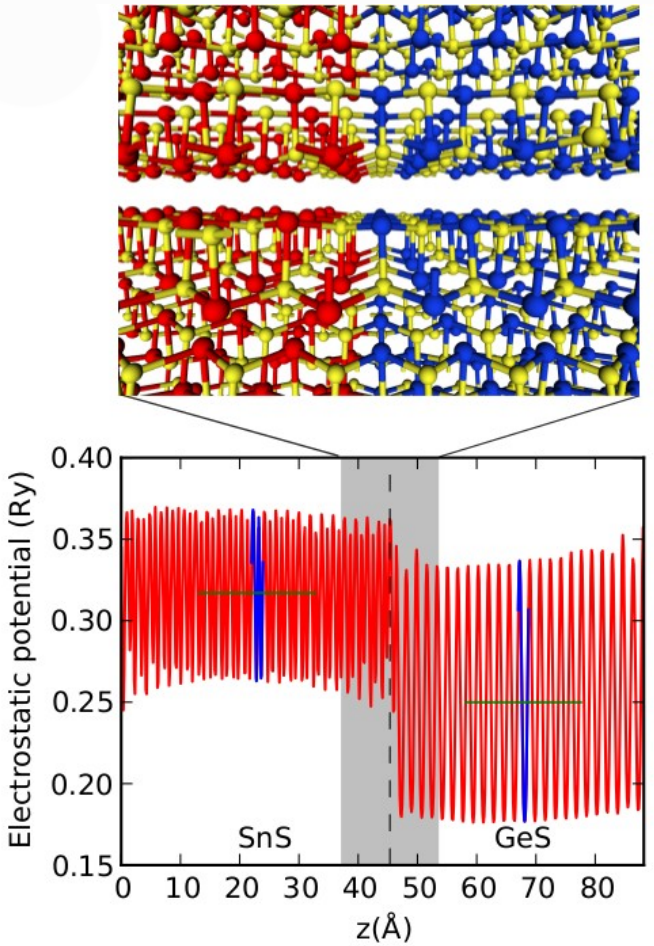
GeS

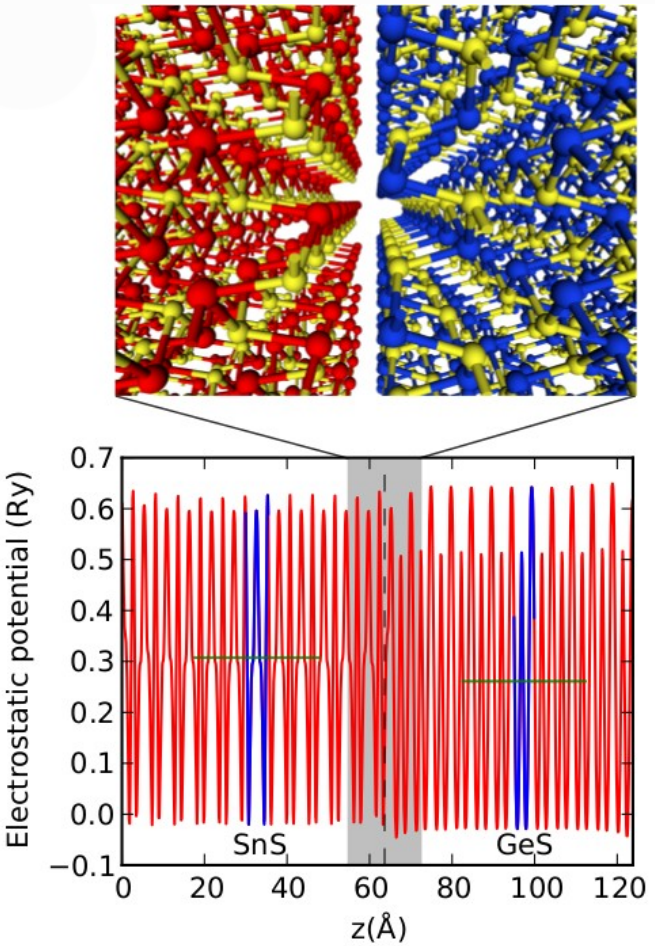
	T(K)	$E_g^{(T)}$(eV)	E_g^0 (eV)
Theory			
Present work			1.74
Ref. [1] (GW)			1.53
Experiment			
Ref. [2]	300	1.65	1.81
Ref. [3]	4.2	1.74	1.75
Ref. [4]	298	1.54	1.70
Ref. [5]	298	1.8	1.96
Ref. [6]	298	1.58	1.74
Ref. [7]	298	1.61	1.74

Ref. [1]: Comp. Mater. Sci., **50**, 2872 (2011)
Ref. [2]: Phys. Rev. B, **16**, 1616 (1977)
Ref. [3]: Solid State Commun., **17**, 355 (1975)
Ref. [4]: J. Phys. C.:Solid State Phys., **21**, 2595 (1988)
Ref. [5]: Semicond. Sci. Technol., **4**, 365 (1989)
Ref. [6]: J. Am. Chem. Soc., **132**, 15170 (2010)
Ref. [7]: J. Phys. Condens. Matter, **2**, 6195 (1990)

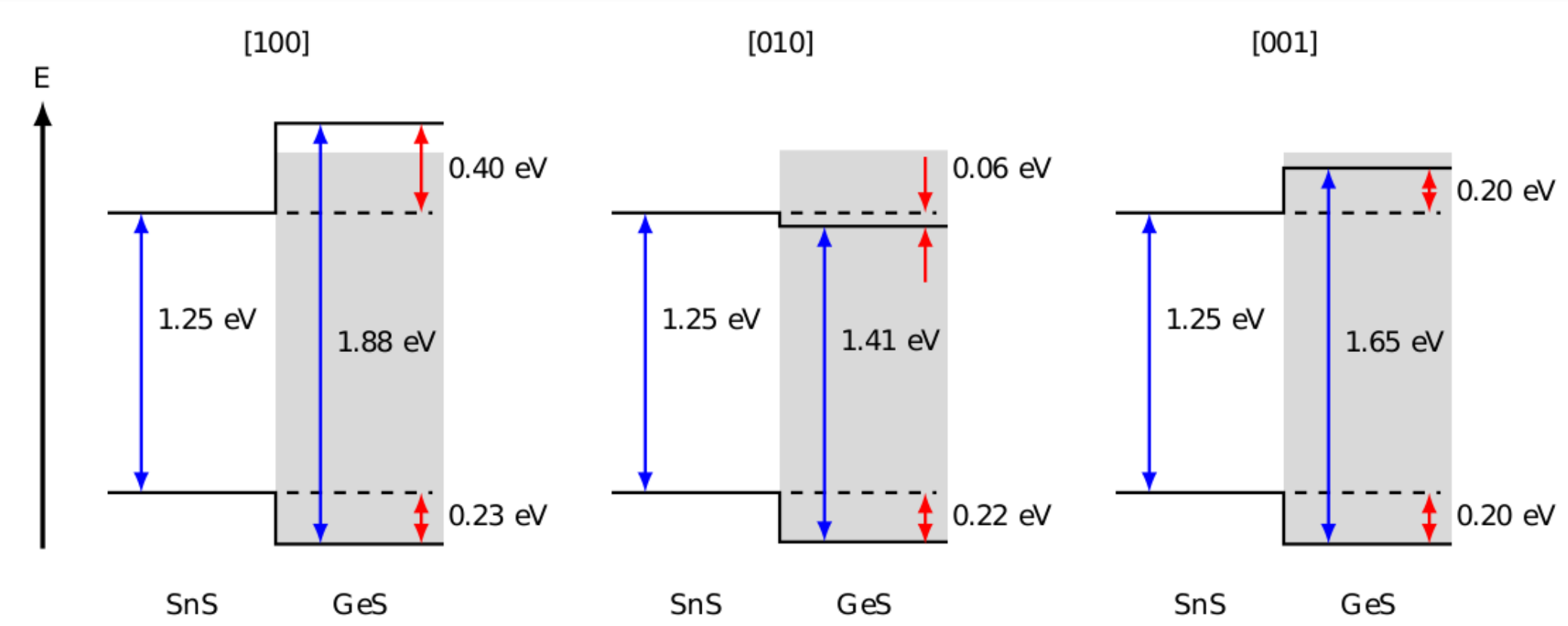
Structural models to determine discontinuity in electrostatic potential caused by interface

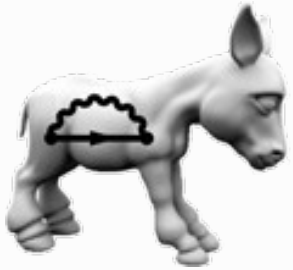






VBOs almost isotropic, CBOs depend strongly on interface orientation





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