Electronic Localization in Semiconductor Alloys

Oleg Rubel & Christopher Pashartis

Department of Materials Science and Engineering

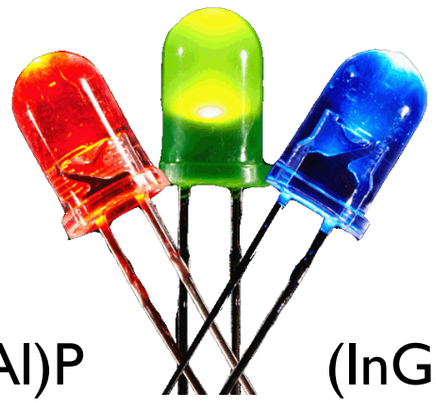
McMaster University

DFT 2017

17th International Conference on Density-Functional Theory and its Applications

Tällberg (Dalarna) Sweden | August 21st – 25th 2017

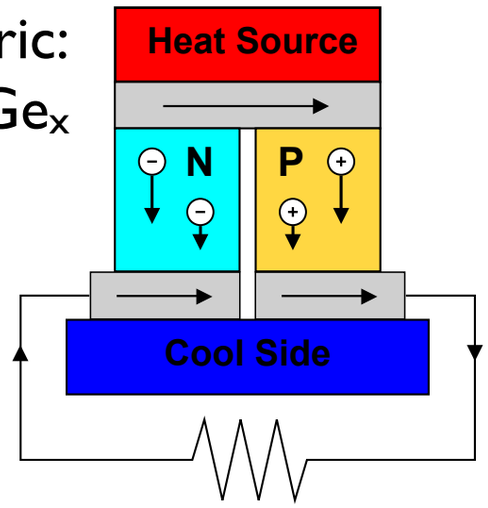
Semiconductor alloys

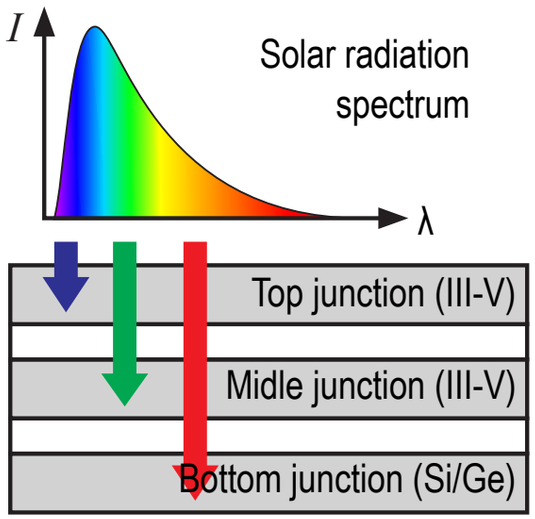


(InGaAl)P (InGa)N

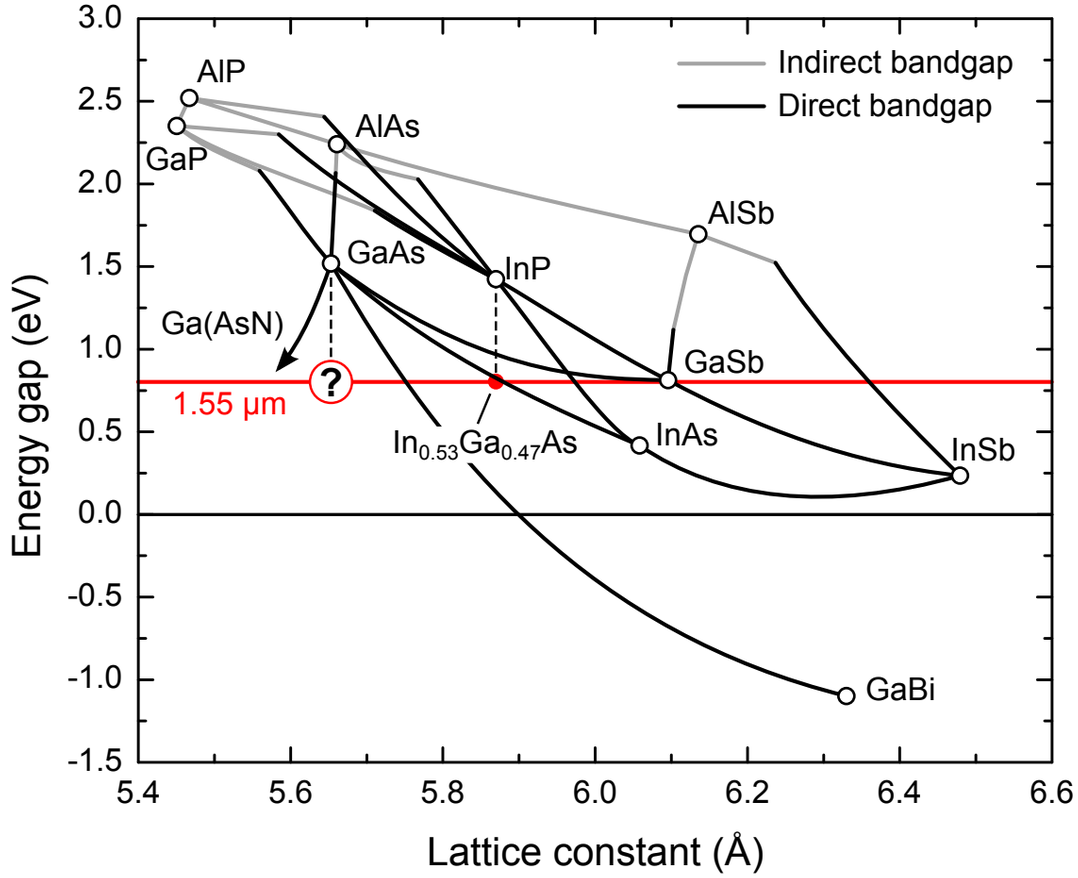
IR detector:
(HgCd)Te

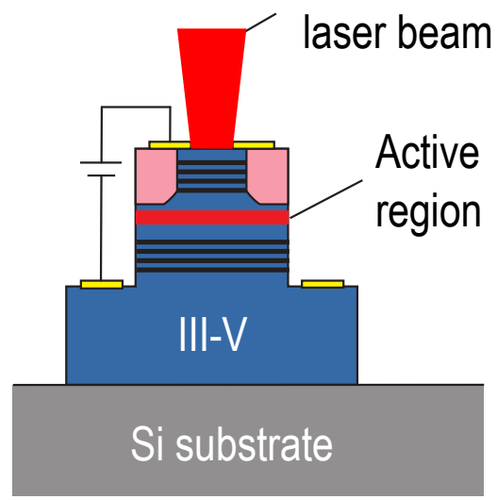
Thermoelectric:
$Si_{1-x}Ge_x$





Eg = 1 eV junction:
(InGa)(NAs)



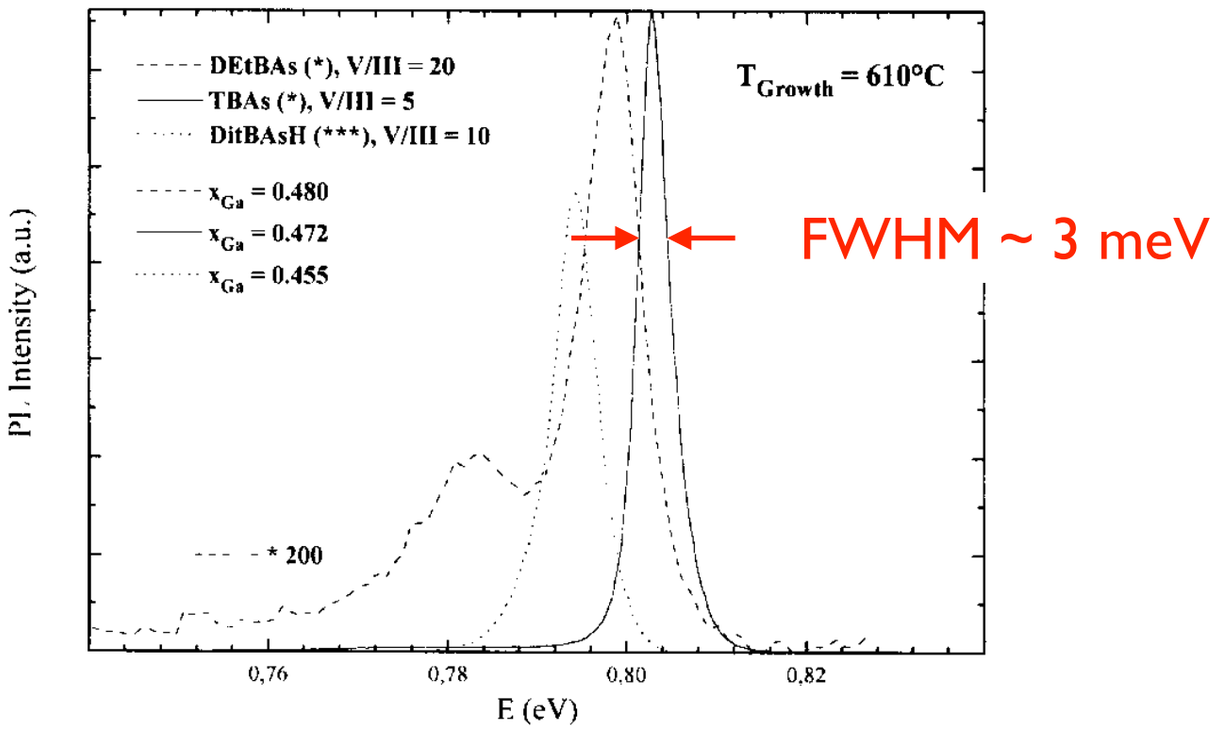


1.55 μm lasers:
(InGa)As
(InGa)(NAsSb)
Ga(AsBi)

Low temperature photoluminescence

$Ga_{1-x}In_xAs$

J. Cryst. Growth **170**, 155 (1997)

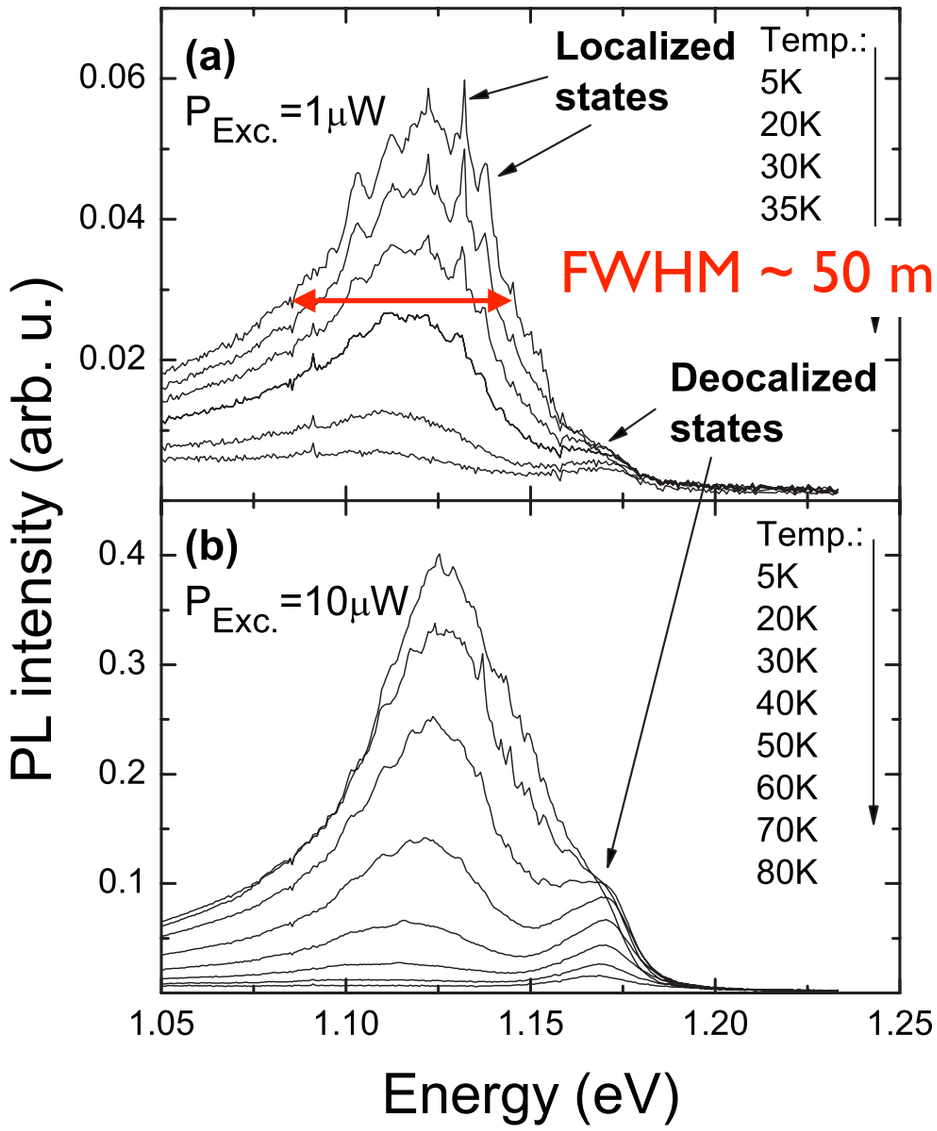


FWHM ~ 3 meV

Fig. 3. Low temperature luminescence spectra of (GaIn)As bulk layers grown by using different As sources as indicated in the inset. The spectrum of the layer grown by using DEtBAs is magnified by a factor of 200.

GaN_xAs_{1-x} $GaBi_xAs_{1-x}$

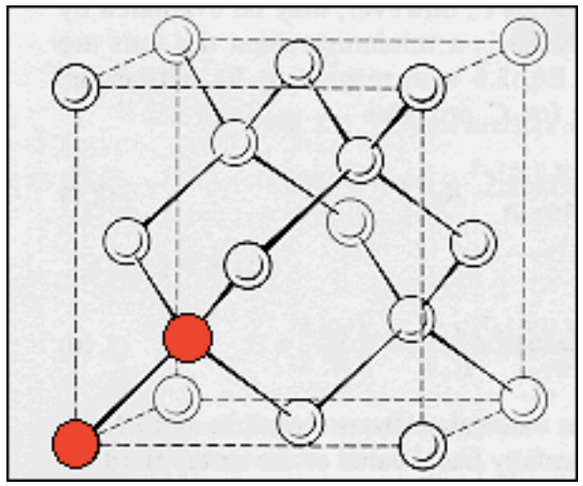
Appl. Phys. Lett. **94**, 011907 (2009)



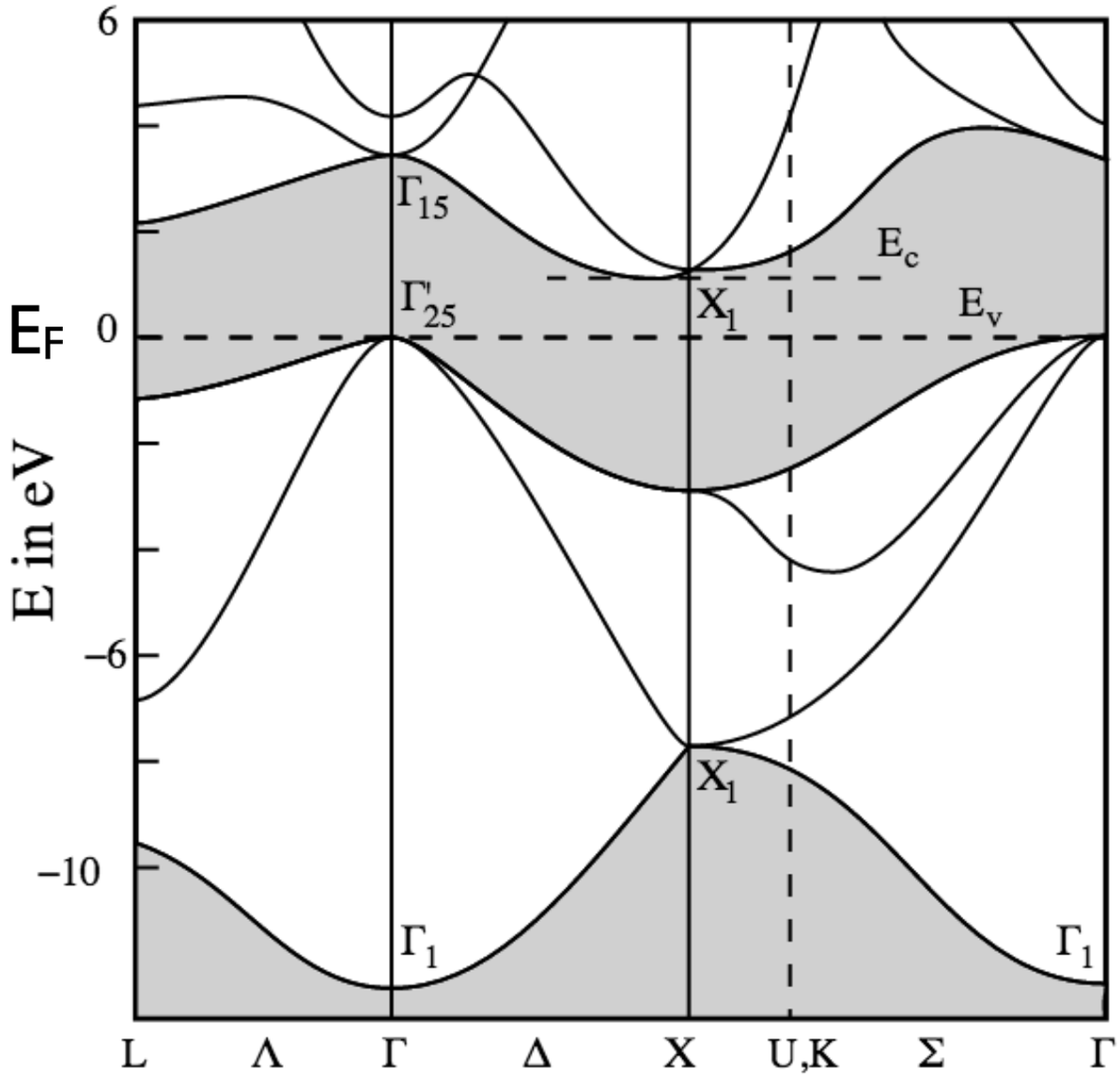
FWHM ~ 50 meV

Inhomogeneous broadening: intrinsic or extrinsic?

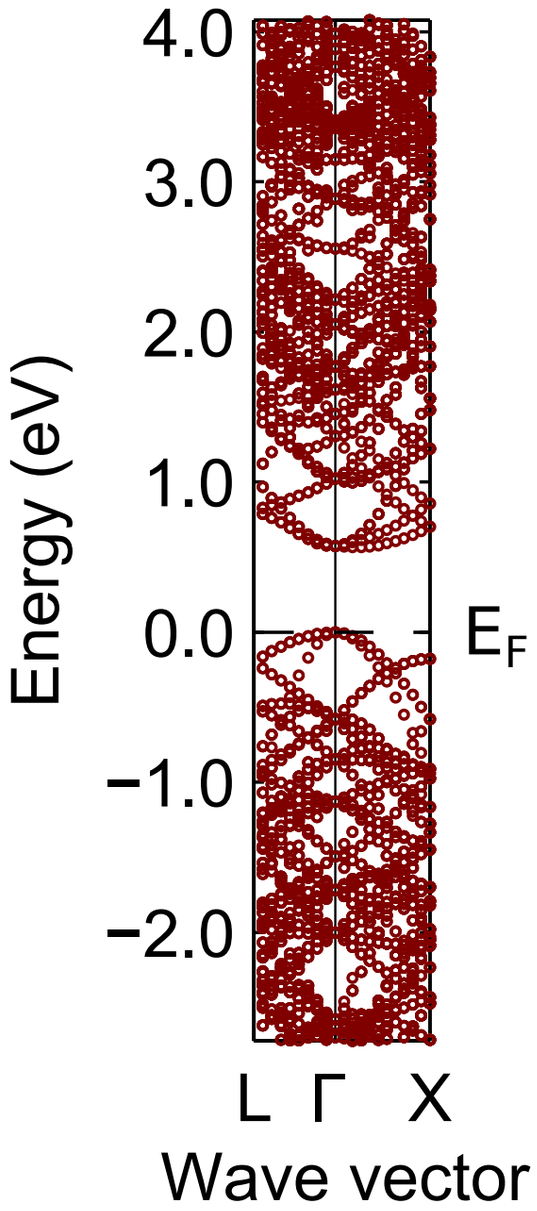
Band structure



Silicon
2-atom basis



Silicon
250-atom supercell



Unfolding the first-principle band structure

Plane wave expansion

$$\Psi_{n,\mathbf{K}}(\mathbf{r}) = \sum_{\mathbf{G}} C_{n,\mathbf{K}}(\mathbf{G})\, \mathrm{e}^{i(\mathbf{K}+\mathbf{G})\cdot\mathbf{r}}$$

Bloch spectral weight

$$w_n(\mathbf{k}) = \sum_{\mathbf{g}} |C_{n,\mathbf{K}}(\mathbf{k}+\mathbf{g})|^2$$

Popescu & Zunger:
Phys. Rev. Lett. **104**, 236403 (2010)

Rubel *et al.*
Phys. Rev. B **90**, 115202 (2014)

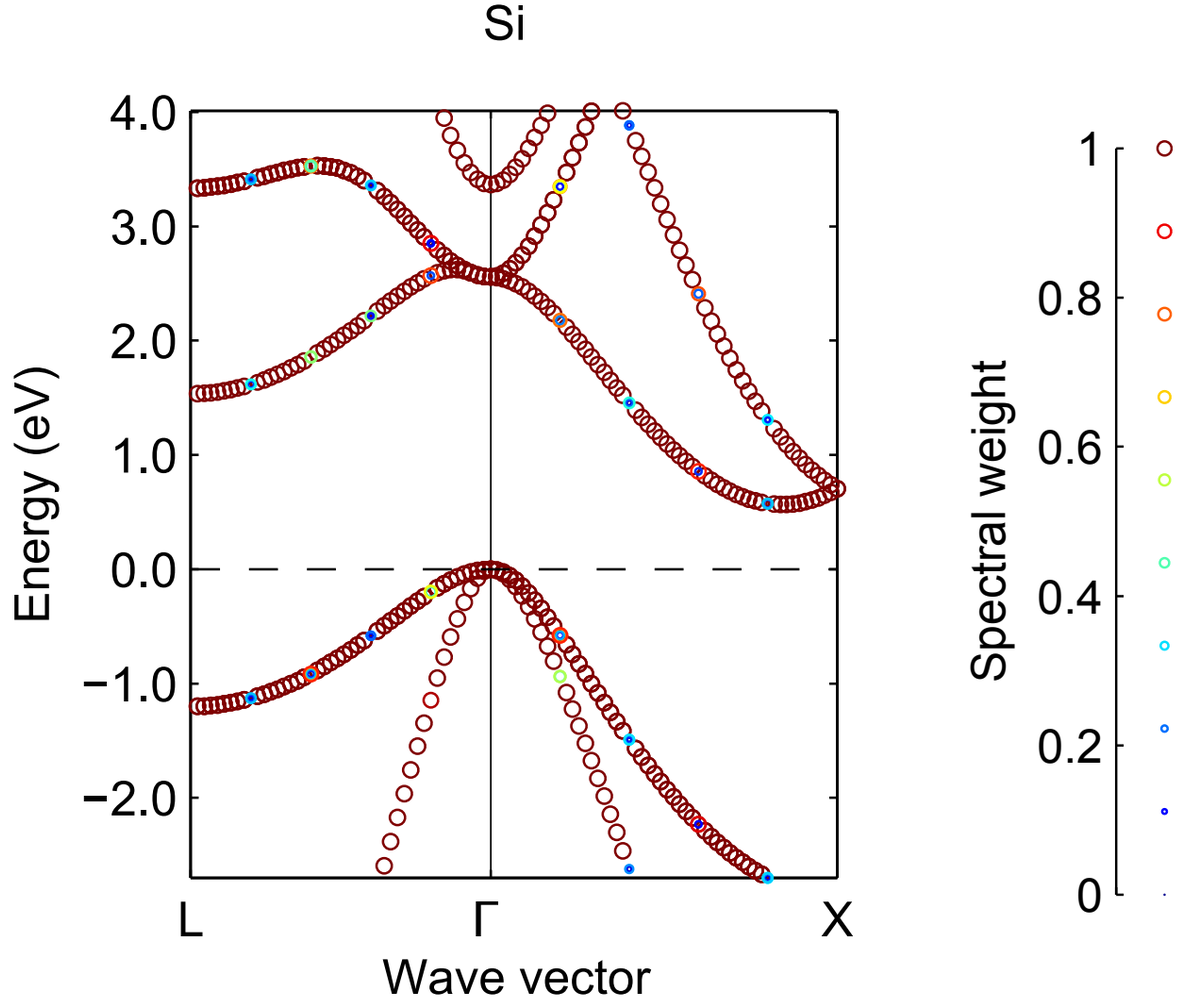
README.md

fold2Bloch

Unfolding of first-principle electronic band structure obtained with WIEN2k DFT-(L)APW code

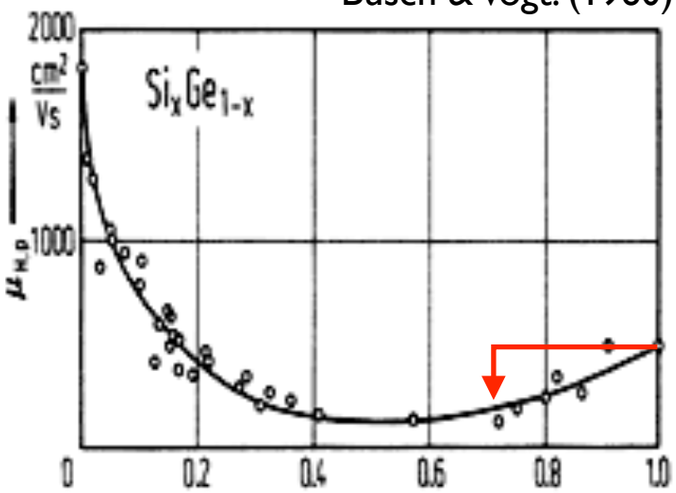
Contributors:

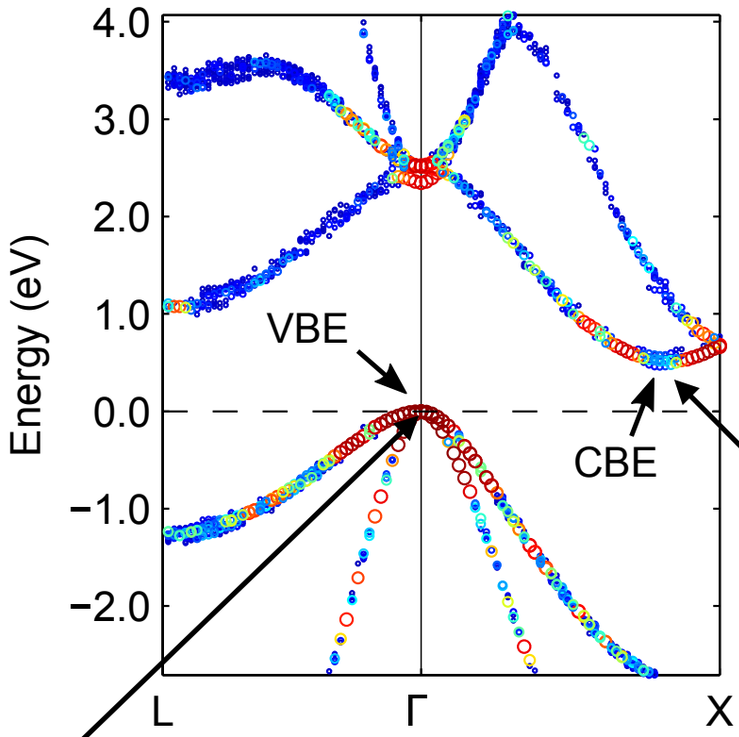
- Anton Bokhanchuk
- Elias Assmann
- Sheikh Jamil Ahmed
- Oleg Rubel

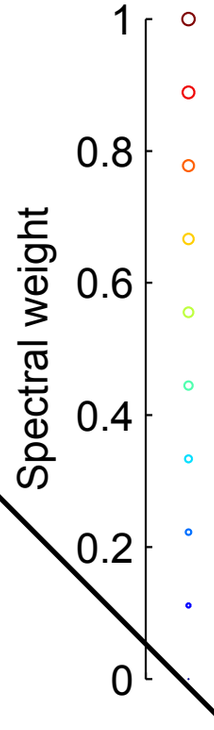


Thermoelectric material: $Si_{0.7}Ge_{0.3}$

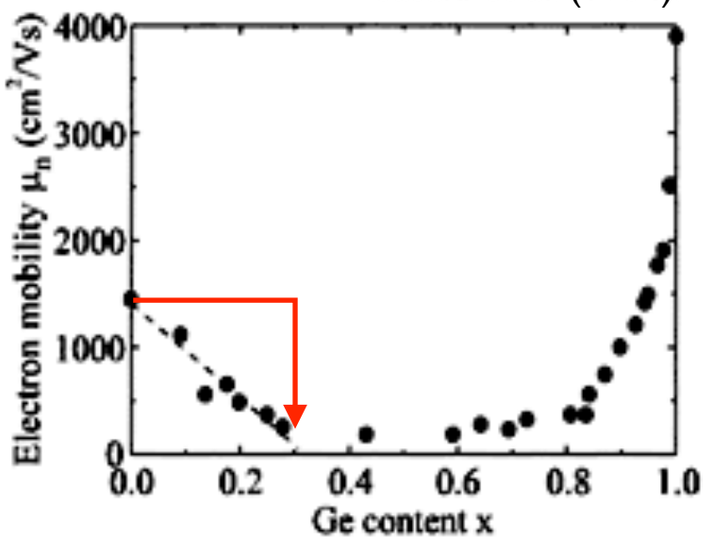
Busch & Vogt. (1960)







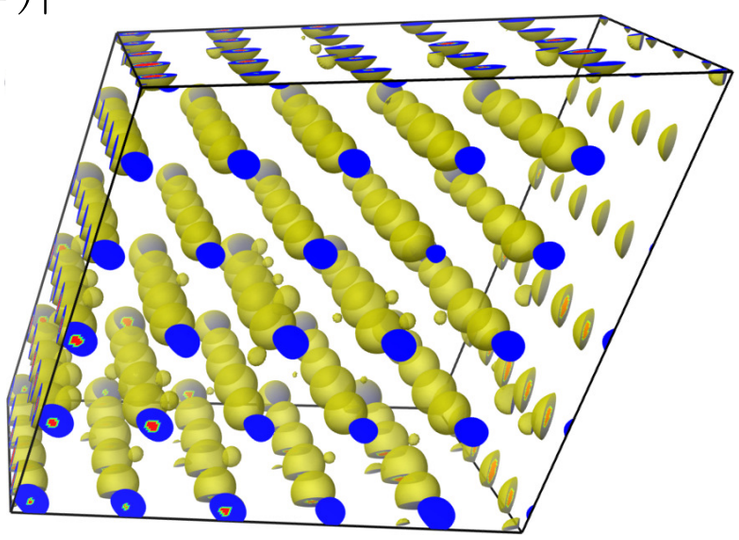
Landoldt-Bornstein (1982, 1987);
Sasaki et al. (1984).



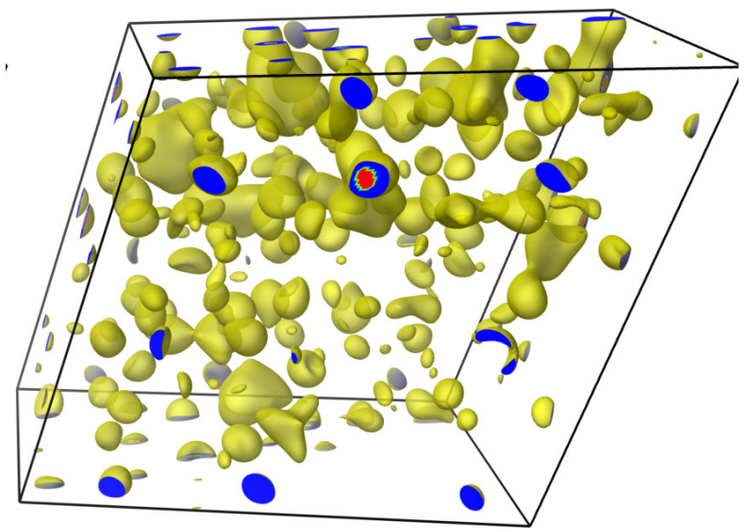
$\Delta r \Delta k \sim 1$

VBE

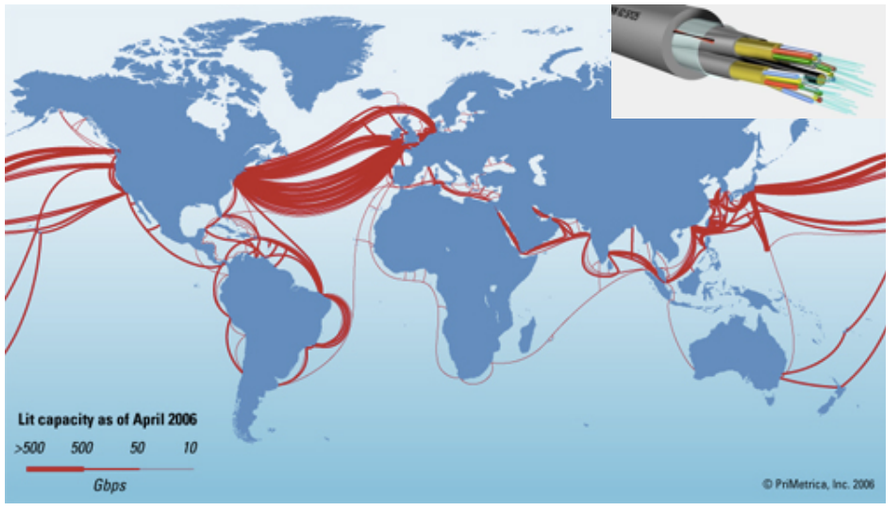
$|\psi(\mathbf{r})|^2$



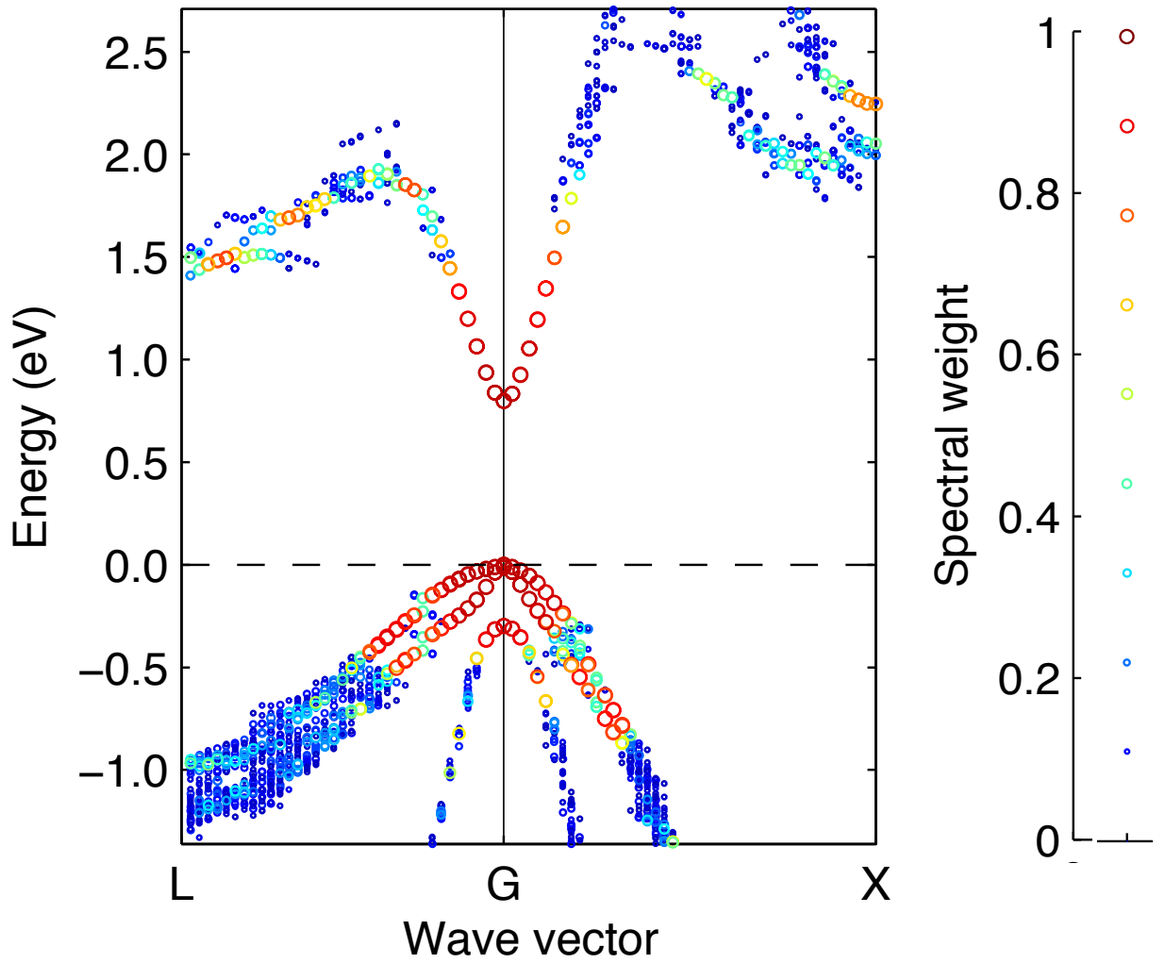
CBE



$In_{0.53}Ga_{0.47}As/InP$

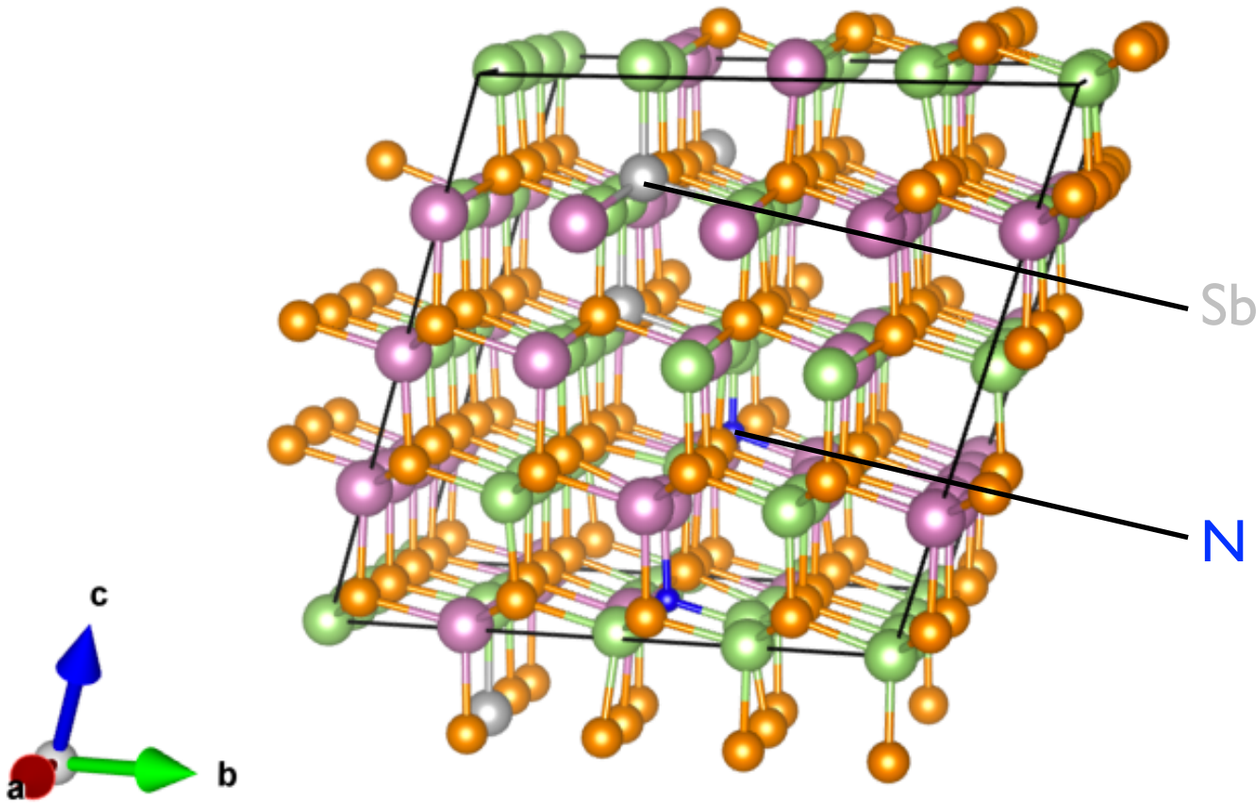


128-atom random alloy models

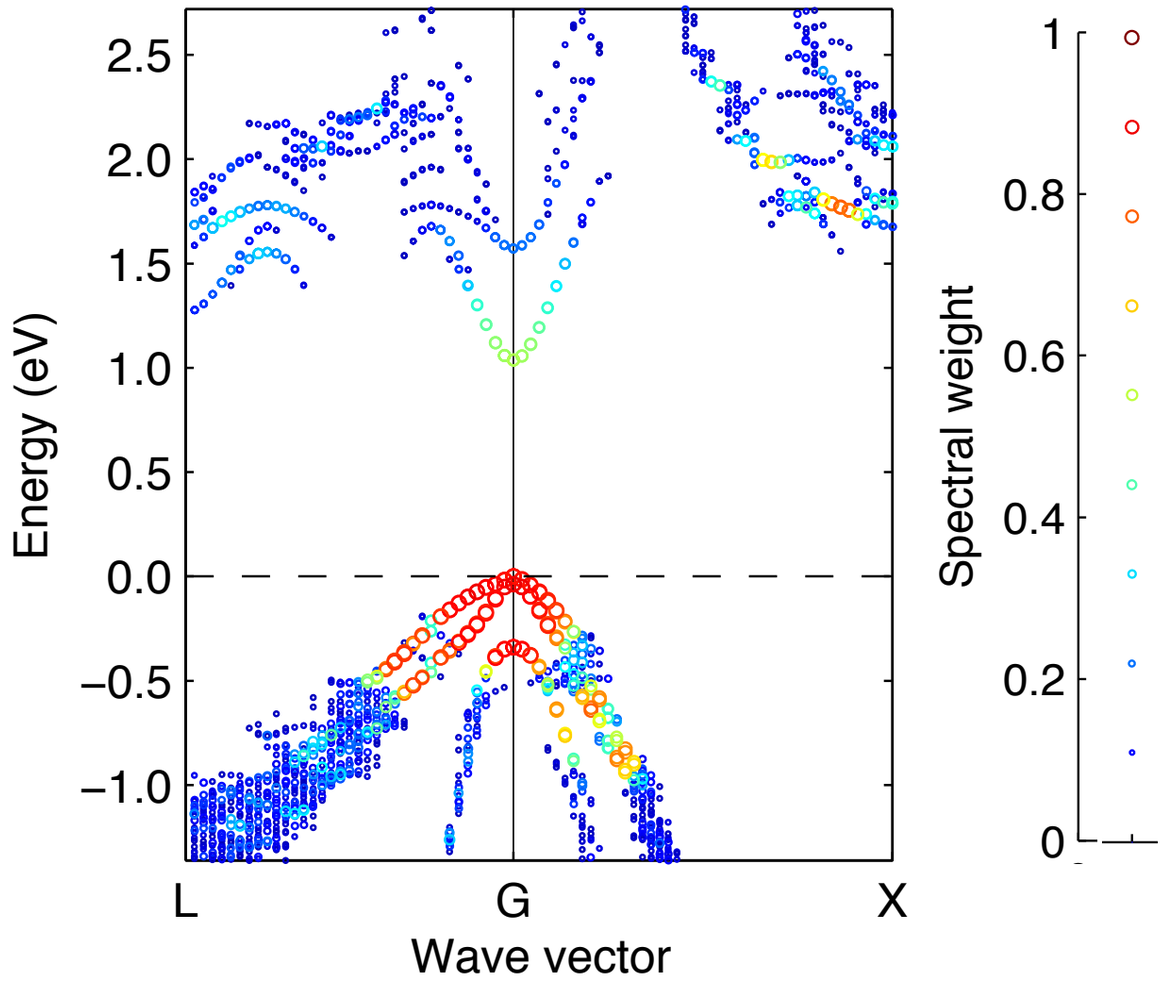


Well preserved Bloch character of the band edges (no localization)

$In_{0.41}Ga_{0.59}N_{0.03}As_{0.94}Sb_{0.03}/GaAs$

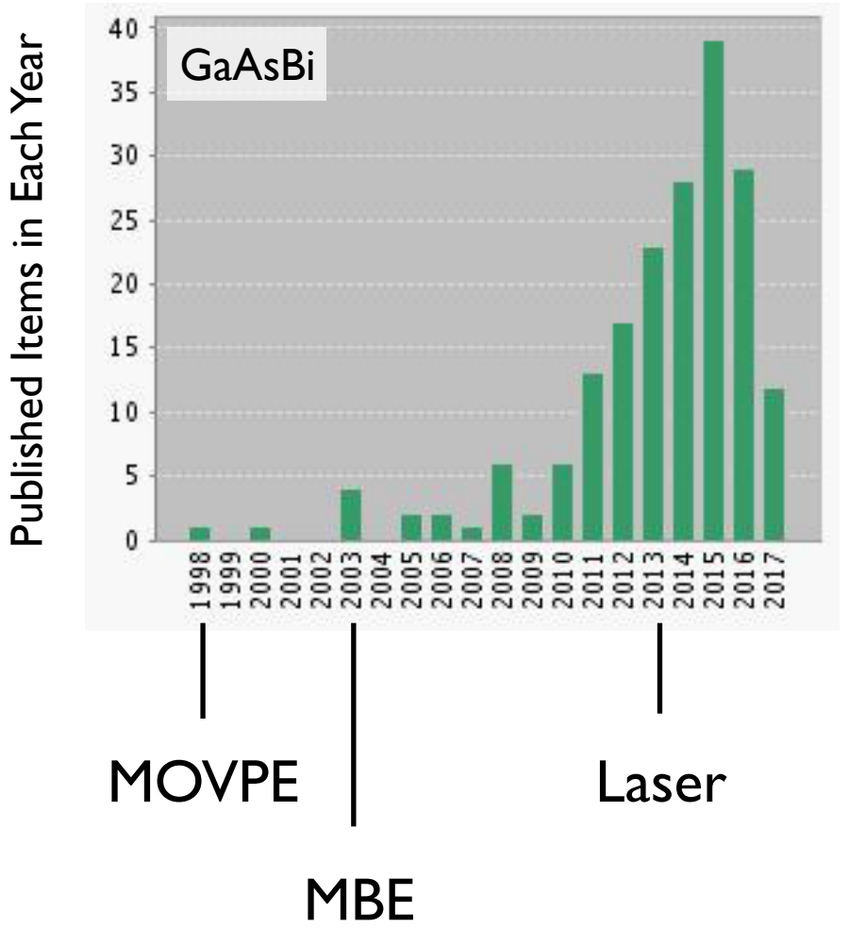


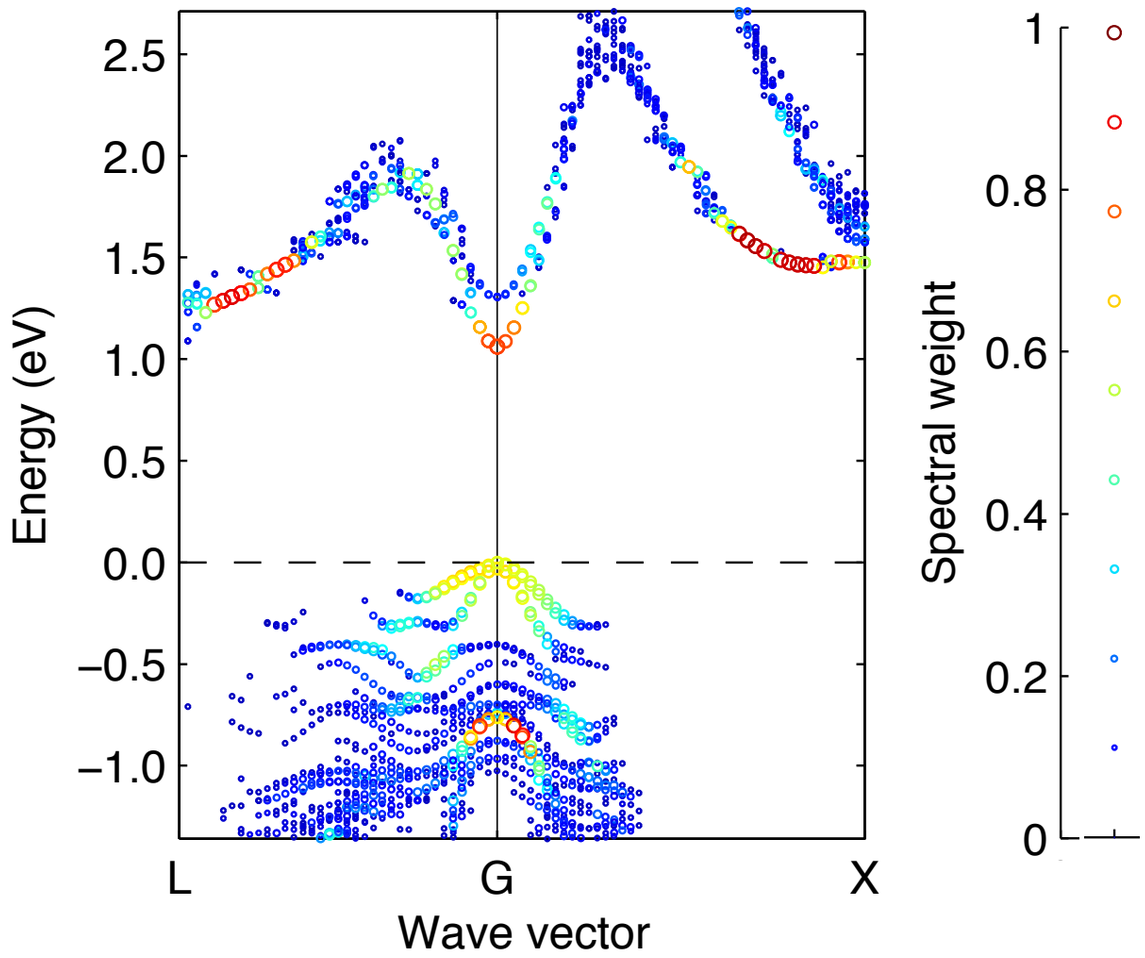
128-atom random alloy models



Large uncertainty in the Bloch character for conduction band edge (localization effects are expected)

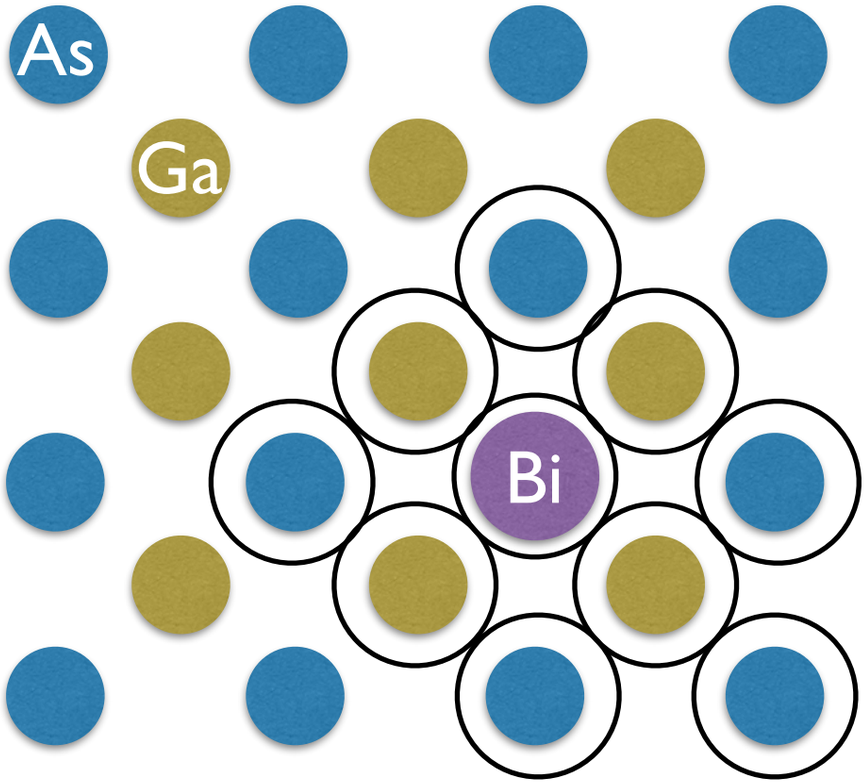
$GaAs_{0.89}Bi_{0.11}/GaAs$





Localization of holes is expected

Inverse participation ratio (IPR)

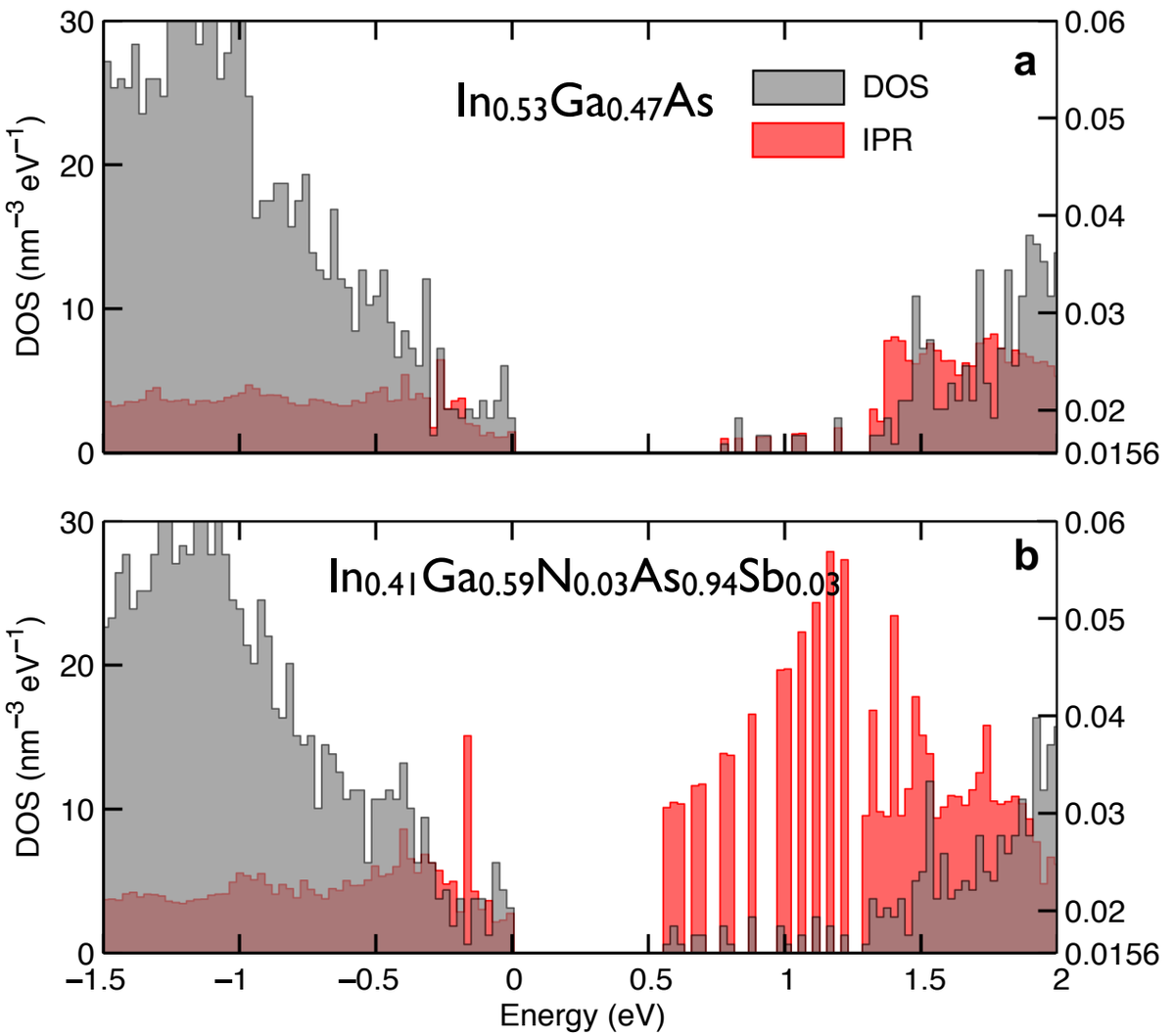


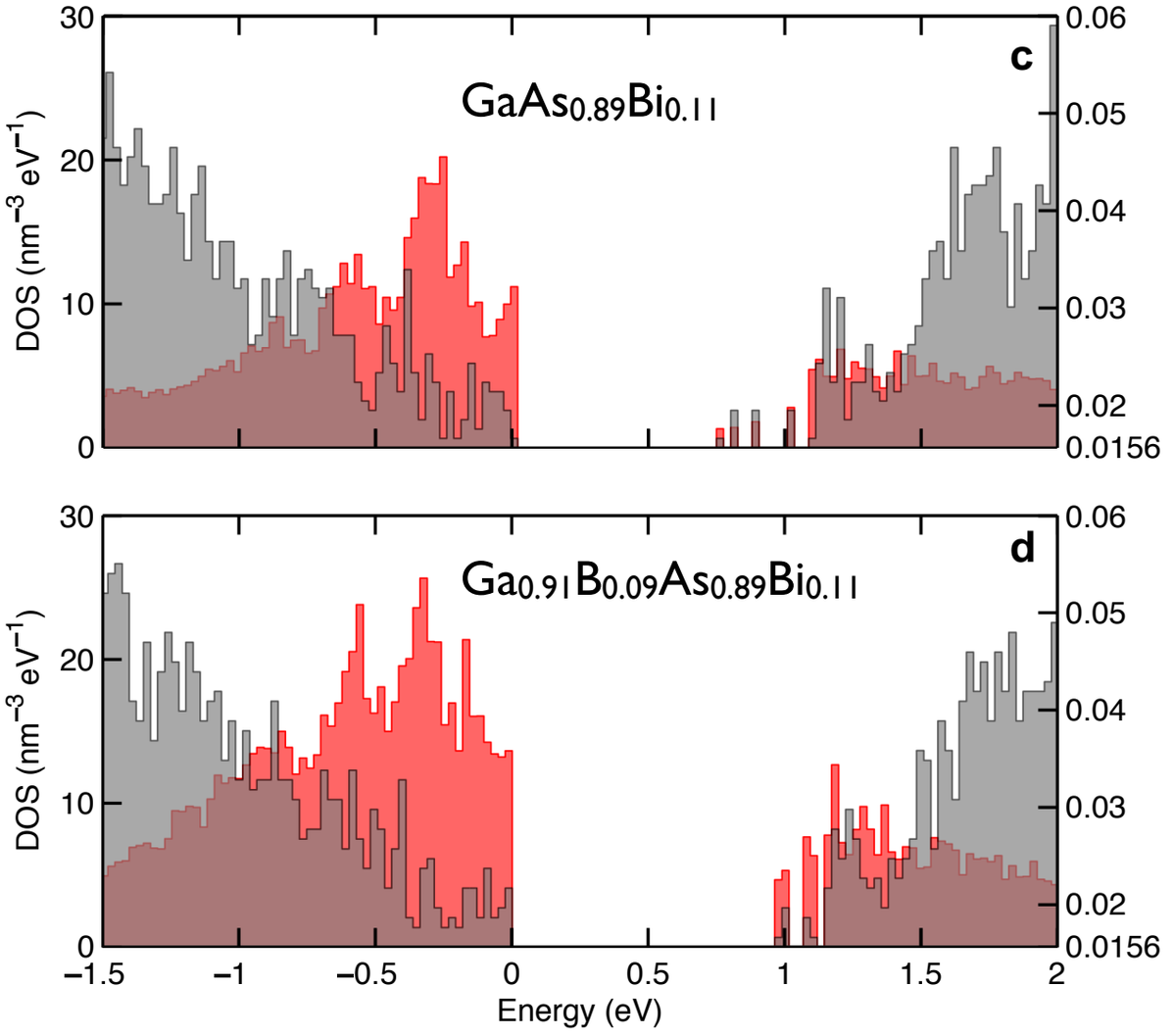
Definition: $\mathrm{IPR}(E_i) = \dfrac{\sum_\alpha \rho_\alpha^2(E_i)}{\left[\sum_\alpha \rho_\alpha(E_i)\right]^2}$

IPR = $1/N_{atoms}$ (no localization)
IPR = 1 (extreme localization)

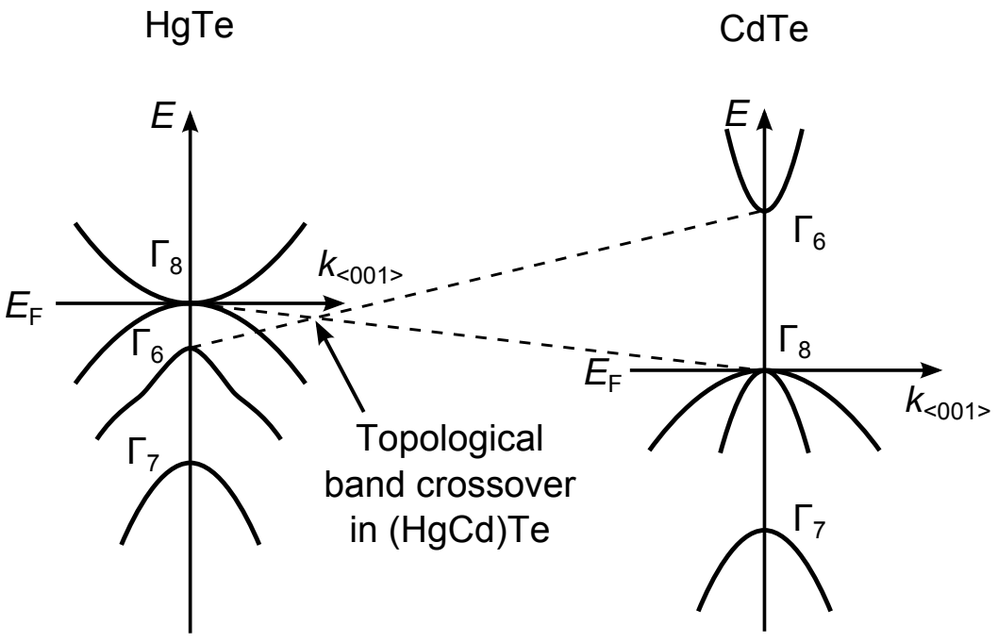
Wegner, Z Physik B **36**, 209 (1980)
Murphy *et al.*, Phys. Rev. B **83**, 184206 (2011)

Localization spectra

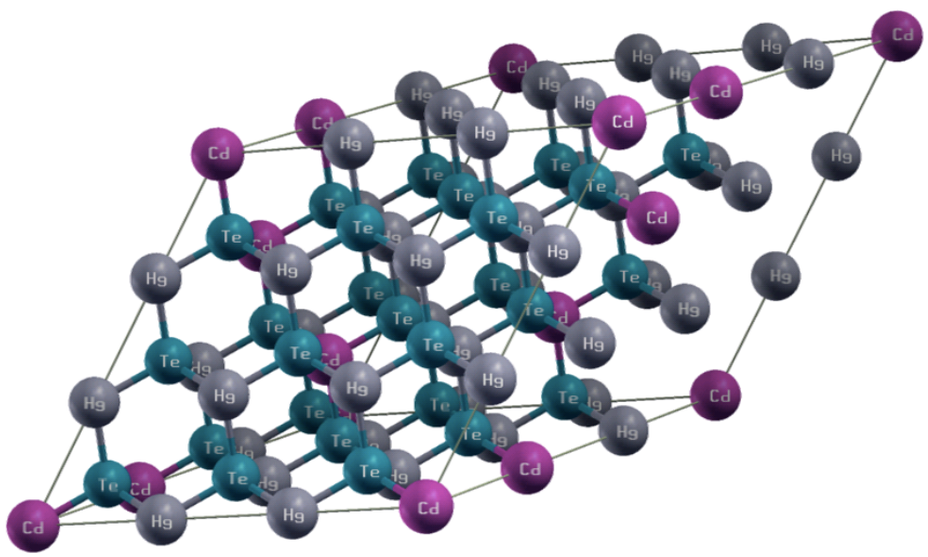


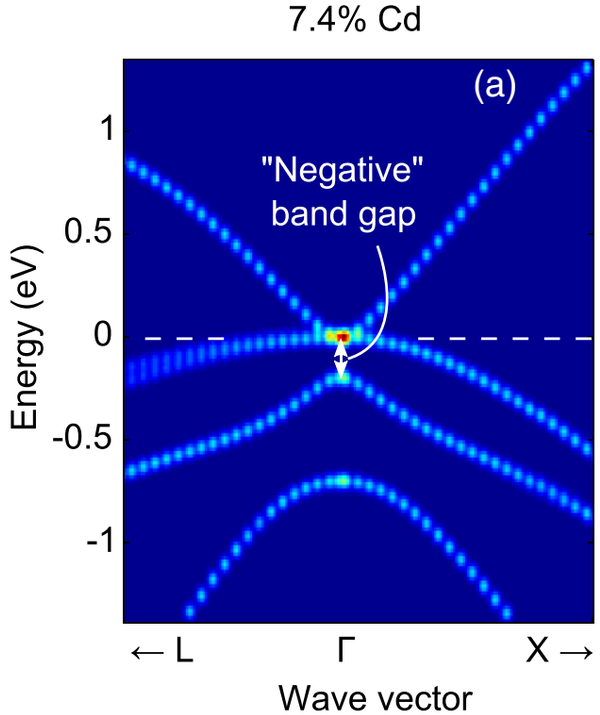


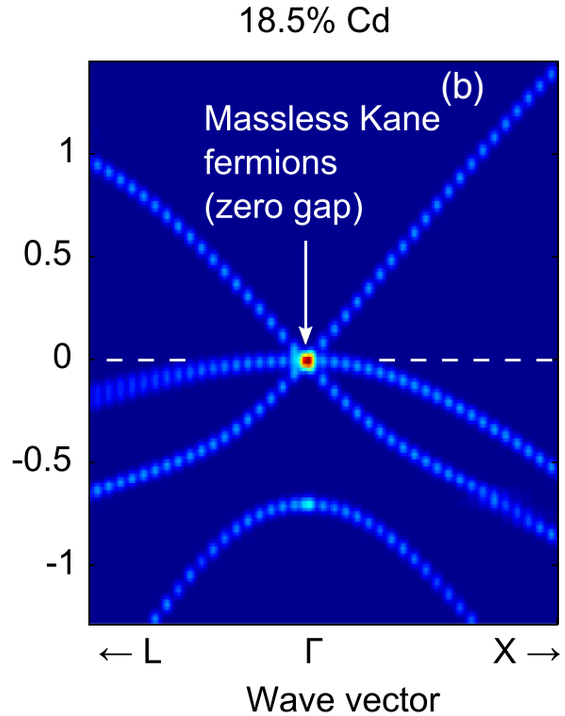
(Hg,Cd)Te band structure evolution

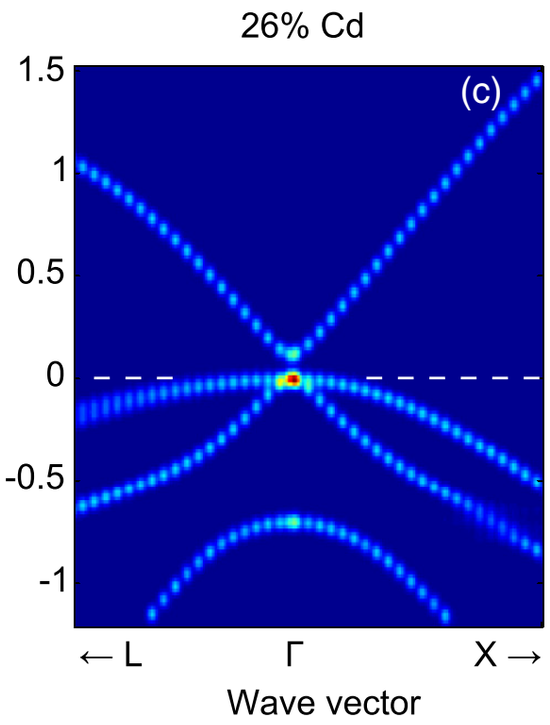


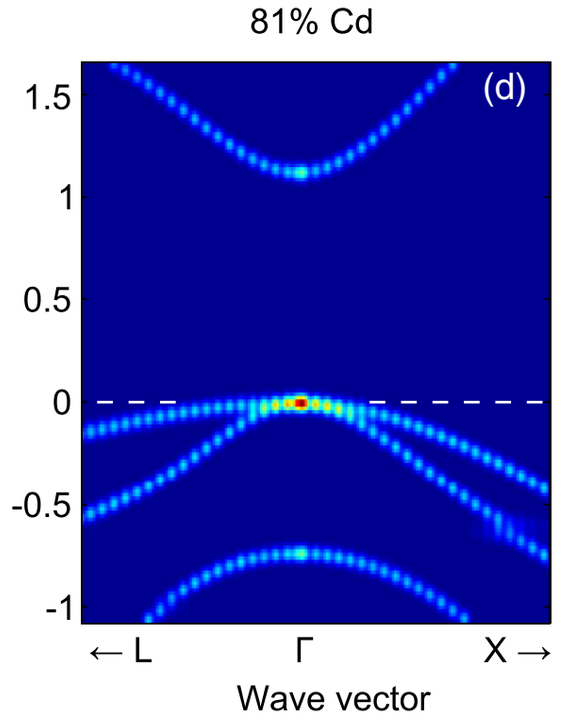
$Hg_{22}Cd_5Te_{27}$





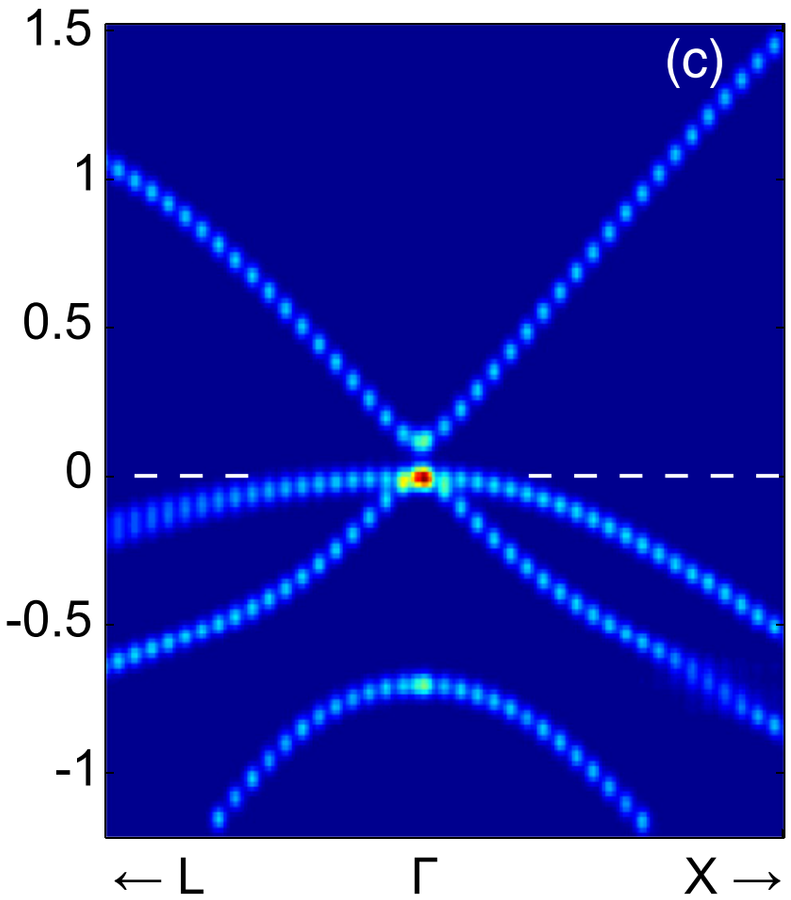






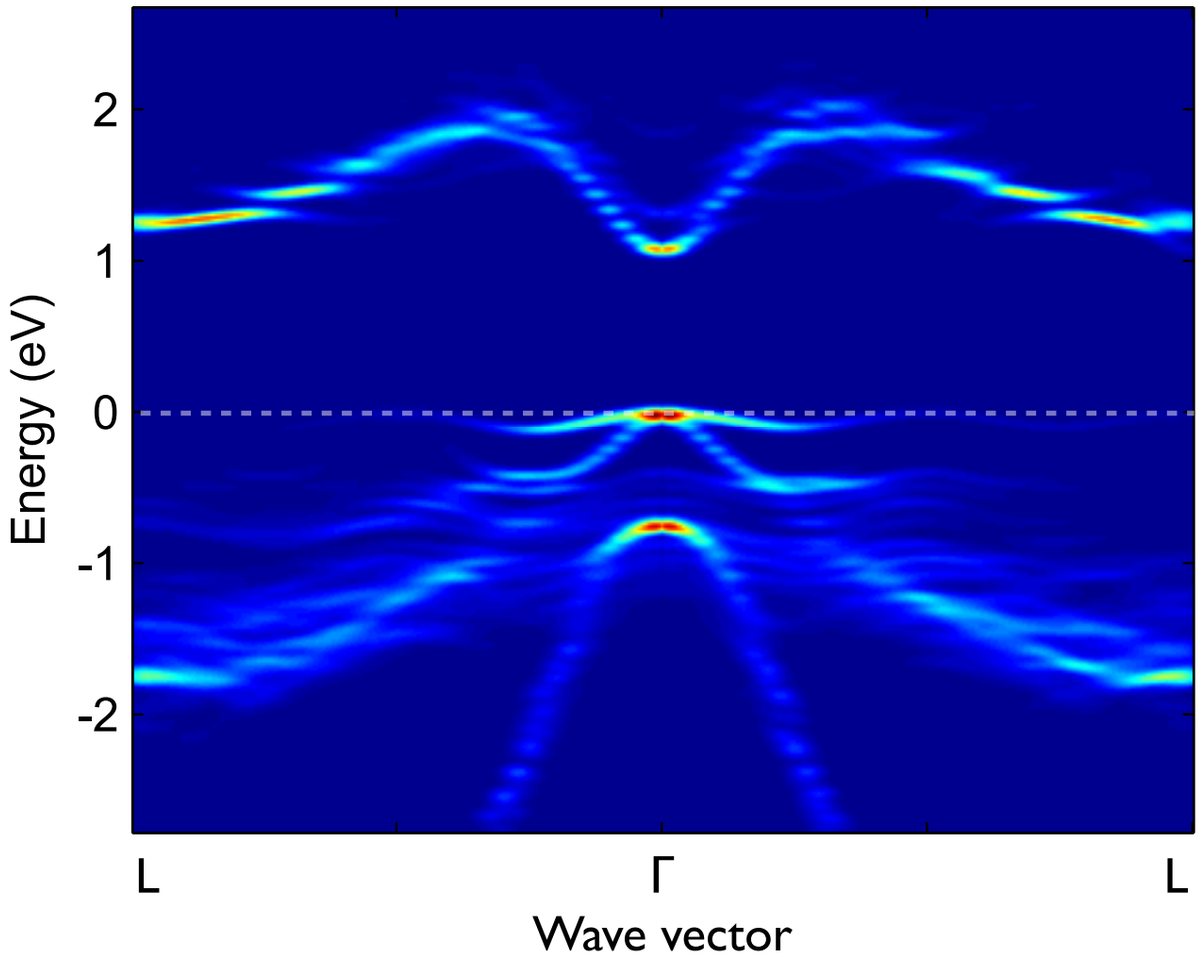
Impact of alloying disorder on charge transport

CdTe → (HgCd)Te



μ_e = 1,100 → 1,000,000 $cm^2V^{-1}s^{-1}$

GaAs → Ga(AsBi)



μ_h = 200 → 10 $cm^2V^{-1}s^{-1}$

μ_e = 4,000 → 2,500 $cm^2V^{-1}s^{-1}$

Summary

	5 **B** Boron 10.811	6 **C** Carbon 12.0107	7 **N** Nitrogen 14.00674	8 **O** Oxygen 15.9994	9 **F** Fluorine 18.9984032
	13 **Al** Aluminum 26.981538	14 **Si** Silicon 28.0855	15 **P** Phosphorus 30.973761	16 Sulfur 32.066	17 Chlorine 35.4527
30 **Zn** Zinc 65.39	31 **Ga** Gallium 69.723	32 **Ge** Germanium 72.61	33 **As** Arsenic 74.92160	34 **Se** Selenium 78.96	35 **Br** Bromine 79.904
48 **Cd** Cadmium 112.411	49 **In** Indium 114.818	50 **Sn** Tin 118.710	51 **Sb** Antimony 121.760	52 **Te** Tellurium 127.60	53 **I** Iodine 126.90447
80 **Hg** Mercury 200.59	81 **Tl** Thallium 204.3833	82 **Pb** Lead 207.2	83 **Bi** Bismuth 208.98038	84 **Po** Polonium (209)	85 **At** Astatine (210)

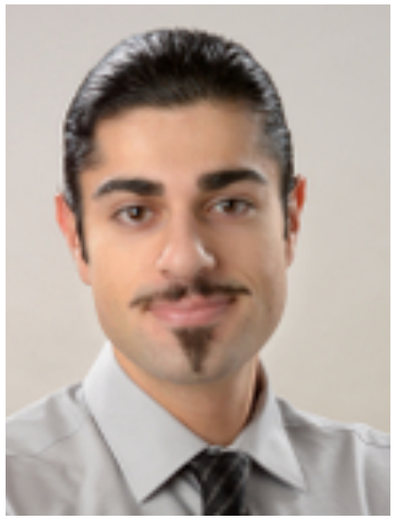
gap one row

- (HgCd)Te
- (InGa)As
- (InGa)(NAsSb) disorder in the conduction band due to electronegative N
- Ga(AsBi) disorder in the valence band due to electropositive Bi

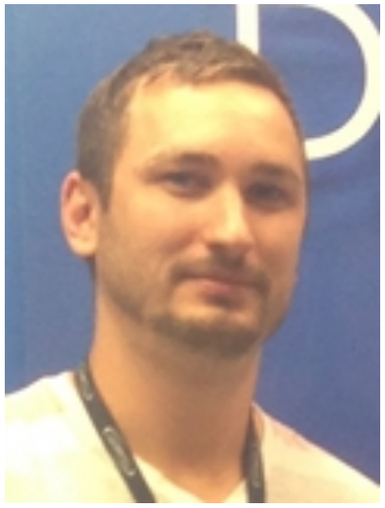
Further reading:

- Phys. Rev. B **90**, 115202 (2014)
- Phys. Rev. Applied **7**, 064011 (2017)
- Comp. Phys. Commun. **205**, 106 (2016)
- Phys. Rev. B **93**, 205202 (2016)
- arXiv:1508.03612
- arXiv:1707.04625

Acknowledgement



Christopher Pashartis (McMaster)



Anton Bokhanchuk (TBRRI/Conf. College)

Elias Assmann (TU Vienna/Uni Graz)

Sheikh J. Ahmed (McMaster/LU/TBRRI)

Marek Niewczas (McMaster)

README.md

fold2Bloch

Unfolding of first-principle electronic band structure obtained with WIEN2k DFT-(L)APW code

Contributors:

- Anton Bokhanchuk
- Elias Assmann
- Sheikh Jamil Ahmed
- Oleg Rubel

Financial support:

NSERC CRSNG