Resolution of the exponent puzzle for the Anderson transition in doped semiconductors

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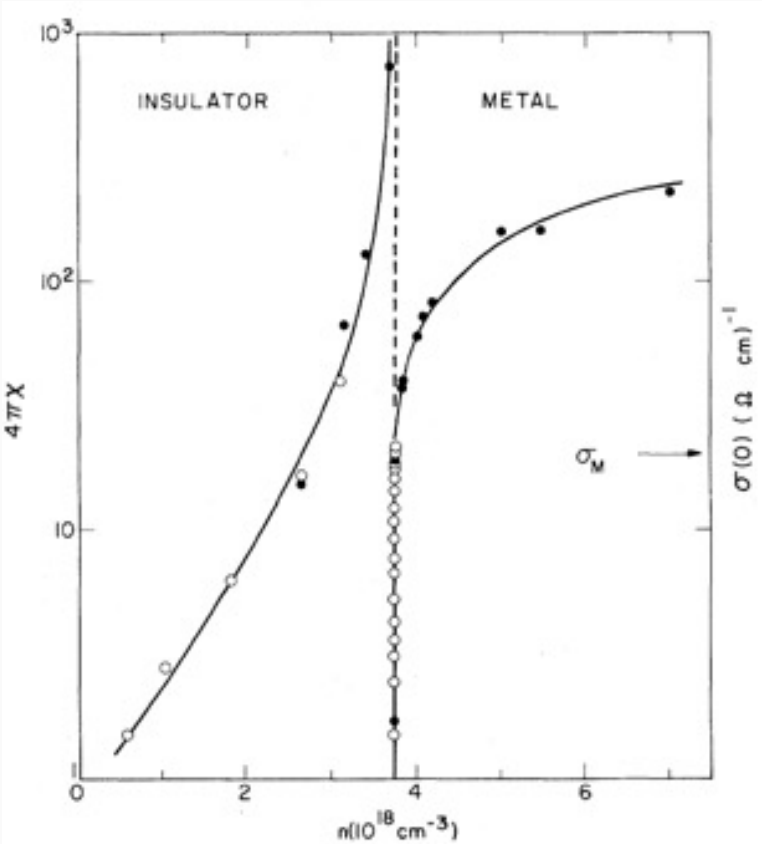
Overview

1. The exponent puzzle
2. Model and analysis
3. Results
4. Conclusions

The exponent puzzle

The exponent puzzle

Doped semiconductors[1]



$$\chi \propto (n_c - n)^{-2\nu} \quad \sigma \propto (n - n_c)^{\nu}$$

Anderson model

$$\mathcal{H} = \sum_i \varepsilon_i |i\rangle \langle i| + \sum_{\langle i,j \rangle} t_{ij} |i\rangle \langle j|$$

with $\varepsilon_i \in \left[-\frac{W}{2}; \frac{W}{2}\right]$ randomly.

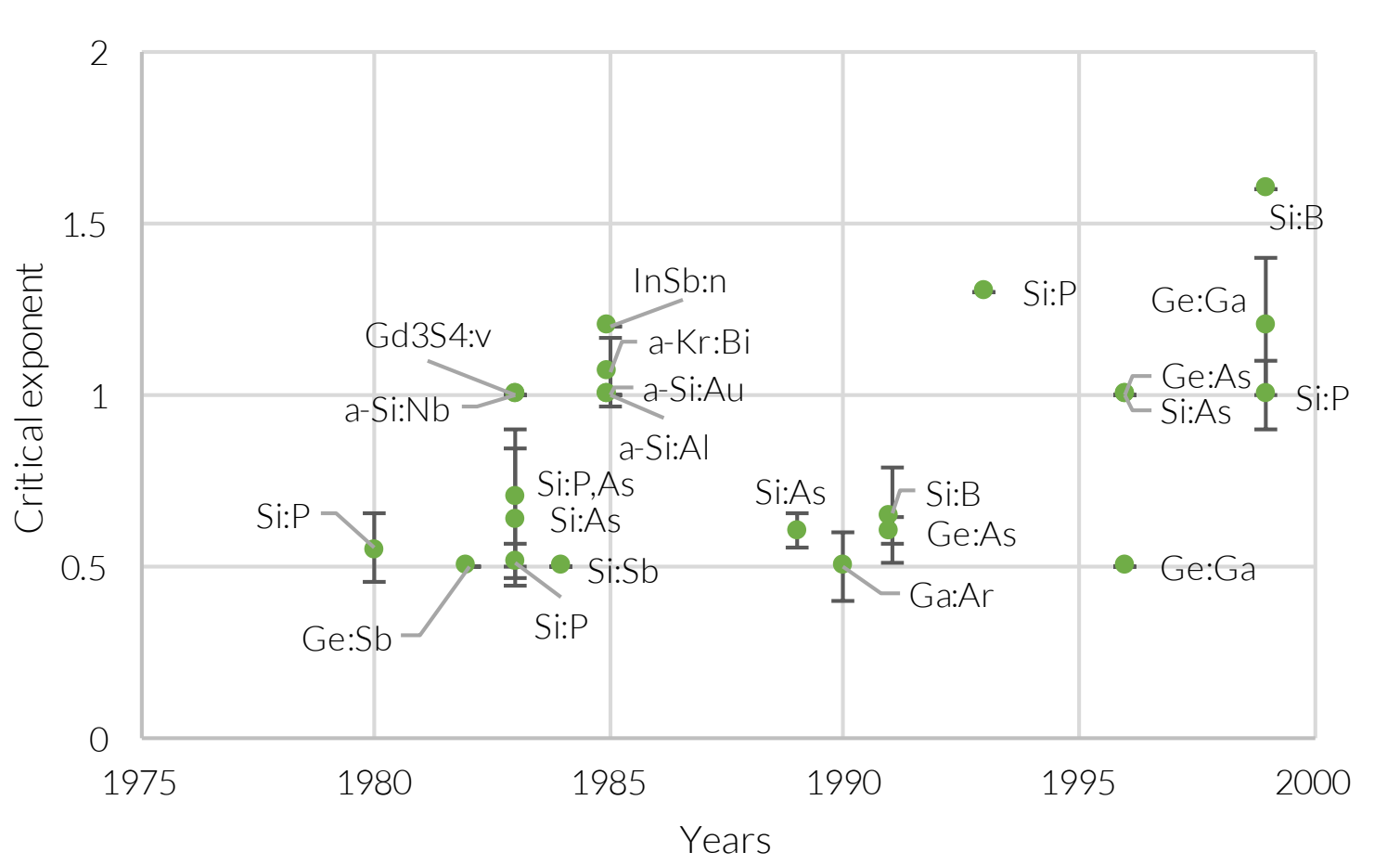
$$\xi \propto |W - W_c|^{-\nu}$$

Critical exponent ν

- Non-interacting[2]: $\nu = 1.590(011)$
- Interacting[3]: $\nu \approx 1.3$ (?)
- Experiments: $\nu \approx 0.5$ to 1

[1] T. F. Rosenbaum et al. *Phys. Rev. B* **1983**, 27, 7509.
[2] A. Rodriguez et al. *Phys. Rev. B* **2011**, 84, 134209.
[3] Y. Harashima and K. Slevin, *Phys. Rev. B* **2014**, 89, 205108.

The exponent puzzle



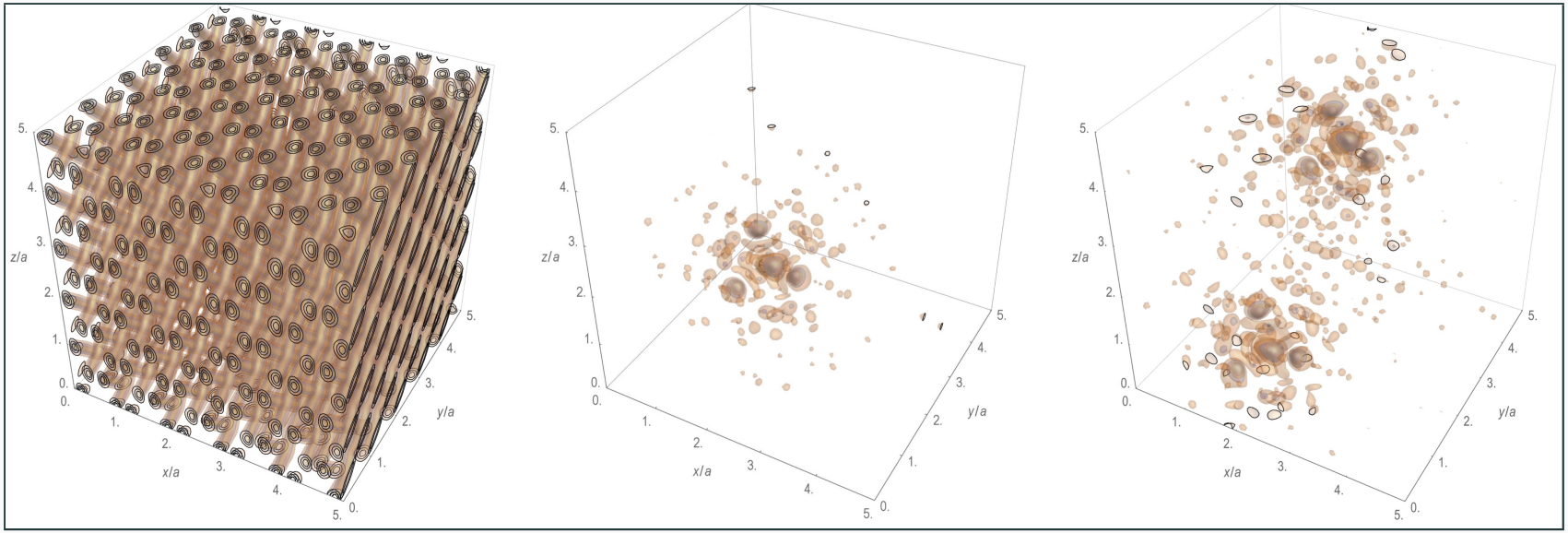
From Thomas[4], Itoh[5] and references therein.

[4] Thomas, G. A. *Philosophical Magazine Part B* **1985**, *52*, 479–498.

[5] Itoh, K. M. et al. *Journal of the Physical Society of Japan* **2004**, *73*, 173–183.

Model and analysis

DFT prototyping



Ab initio description of S-doped Si with DFT (ONETEP[6]):

- host lattice (diamond cubic)
- 9 atomic orbitals (s, p, d)
- interactions via XC functional

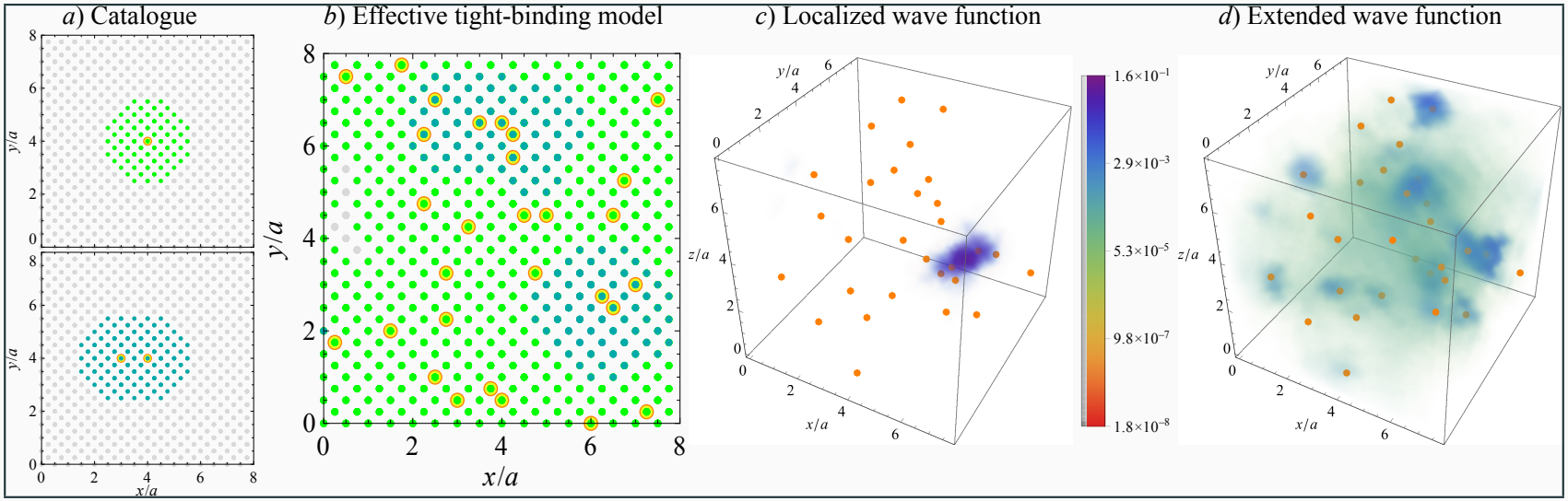
$\Rightarrow$ Observe the MIT via the Kohn-Sham wave function.

ONETEP on ARCHER

4096 atoms = 10h $\times$ 1152 cores.

[6] C.-K. Skylaris et al. *J. Chem. Phys.* **2005**, 122, 084119.

From DFT to effective tight-binding models



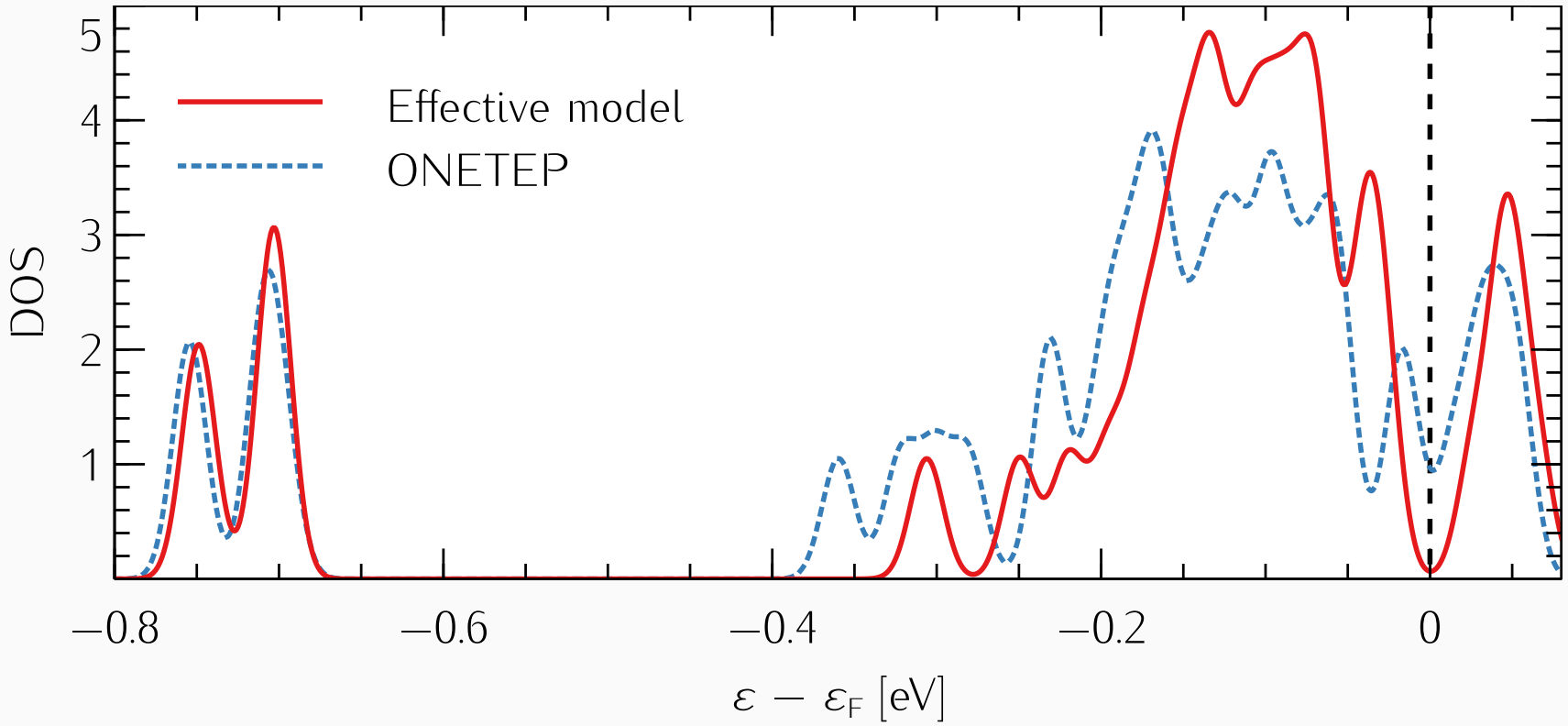
Assumptions and features:

- same potential (matrix elements) around each impurity;
- hopping up to ten neighbours ($\sim 1.6a$), determined by DFT;
- we consider single and paired impurities ($\leq a$).

Model keeps salient features of DFT: single electron at $T = 0$, interacting with other electrons and nuclei via the "Coulomb interaction" (approximated in the XC functional).

An example: 4067Si29S

Diagonalise ETBM to find eigenvalues ε_i. DOS: sum Gaussians centred on $\varepsilon_i - \varepsilon_F$ of width $\sigma = 10\,\text{meV}$.



Good agreement for the position of *conduction* and *valence band* and for the extension of the *impurity band*.

The workflow

1. Generate a disorder realisation.
   Place randomly N_X impurities in a lattice of $N = L^3$ atoms. We work with 4096, 5832, 8000 and 10648 atoms.
2. Construct Hamiltonian H and overlap S matrices.
   They contain the tight-binding model and orbital description. Matrix sizes up to $10648 \times 9 = 95832$, sparsity of ˜600 elements per row.
3. Generalised eigenvalue problem $H\psi_i = \lambda_i S\psi_i$, for $i = 1, \ldots, N_X$.
   For a given concentration $n \propto N_X/N$ the number of eigenstates increases as $N_X \propto N$. Runtime: up to ˜12+ h for 10648 atoms.
4. From the eigenvalues compute the DOS and from the eigenstates compute the multifractal analysis.
   Our statistics is based on ˜18×10^6 eigenstates!

Multifractal analysis[2]

1. Coarse-grain wave function from ψ (sites i in cube L^3) to μ (boxes k in cube $(L/l)^3$):

$$\lambda = l/L \qquad |\psi_i|^2 \to \mu_k = \sum_{i \in \mathcal{B}_k} |\psi_i|^2 \tag{1}$$

2. Compute multifractal exponents:

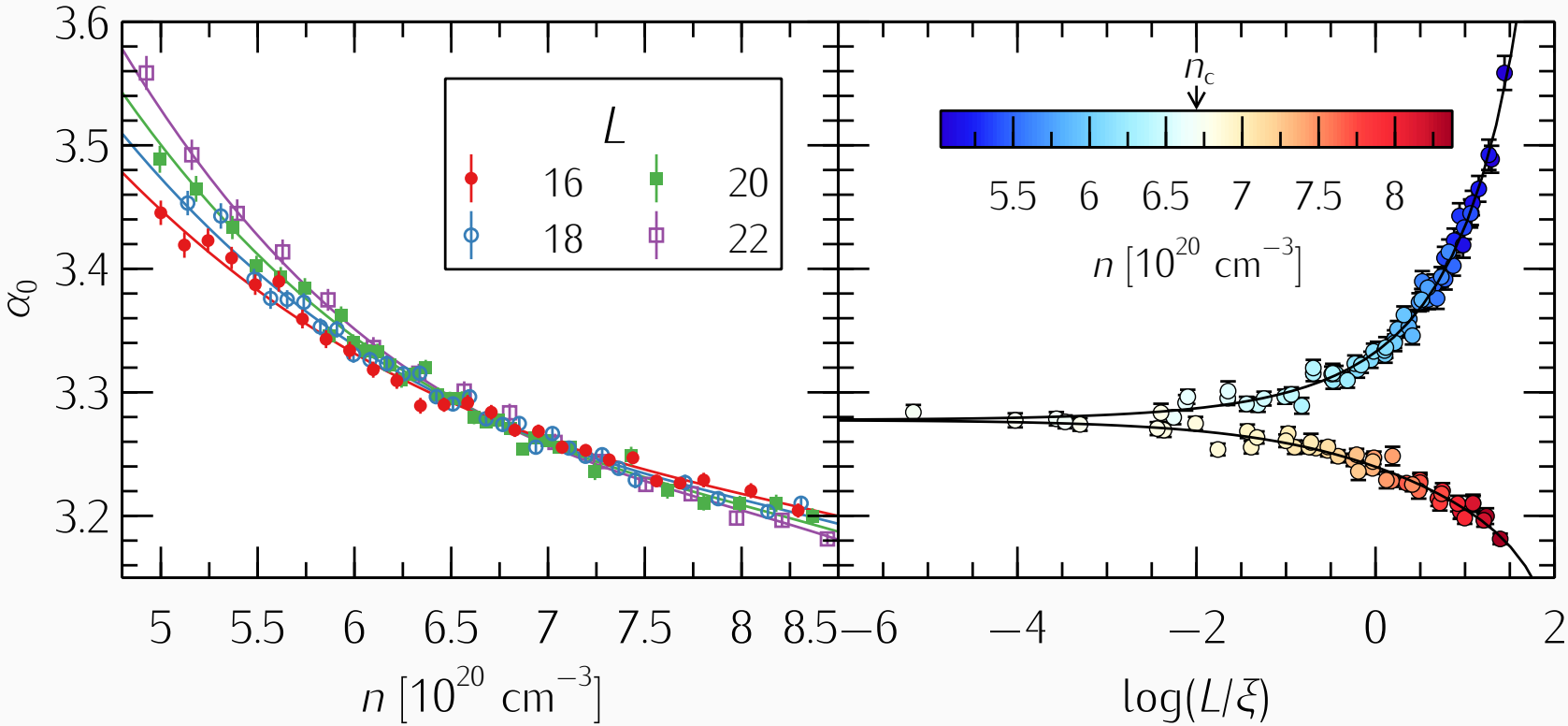
$$\alpha_q = \frac{1}{\ln \lambda} \frac{\sum_i \mu_i^q \ln \mu_i}{\sum_i \mu_i^q} \qquad \tau_q = \frac{\ln \left(\sum_i \mu_i^q\right)}{\ln \lambda} \qquad f_q = q\alpha_q - \tau_q \tag{2}$$

3. Average over the ensemble of realisations.
4. Study the scaling with L and n.

[2] A. Rodriguez et al. *Phys. Rev. B* **2011**, 84, 134209.

Finite-size scaling[2]

$\lambda = l/L = 1/2$ $\varepsilon - \varepsilon_F = -0.25\,\mathrm{eV}$ ~700-1000 realisations

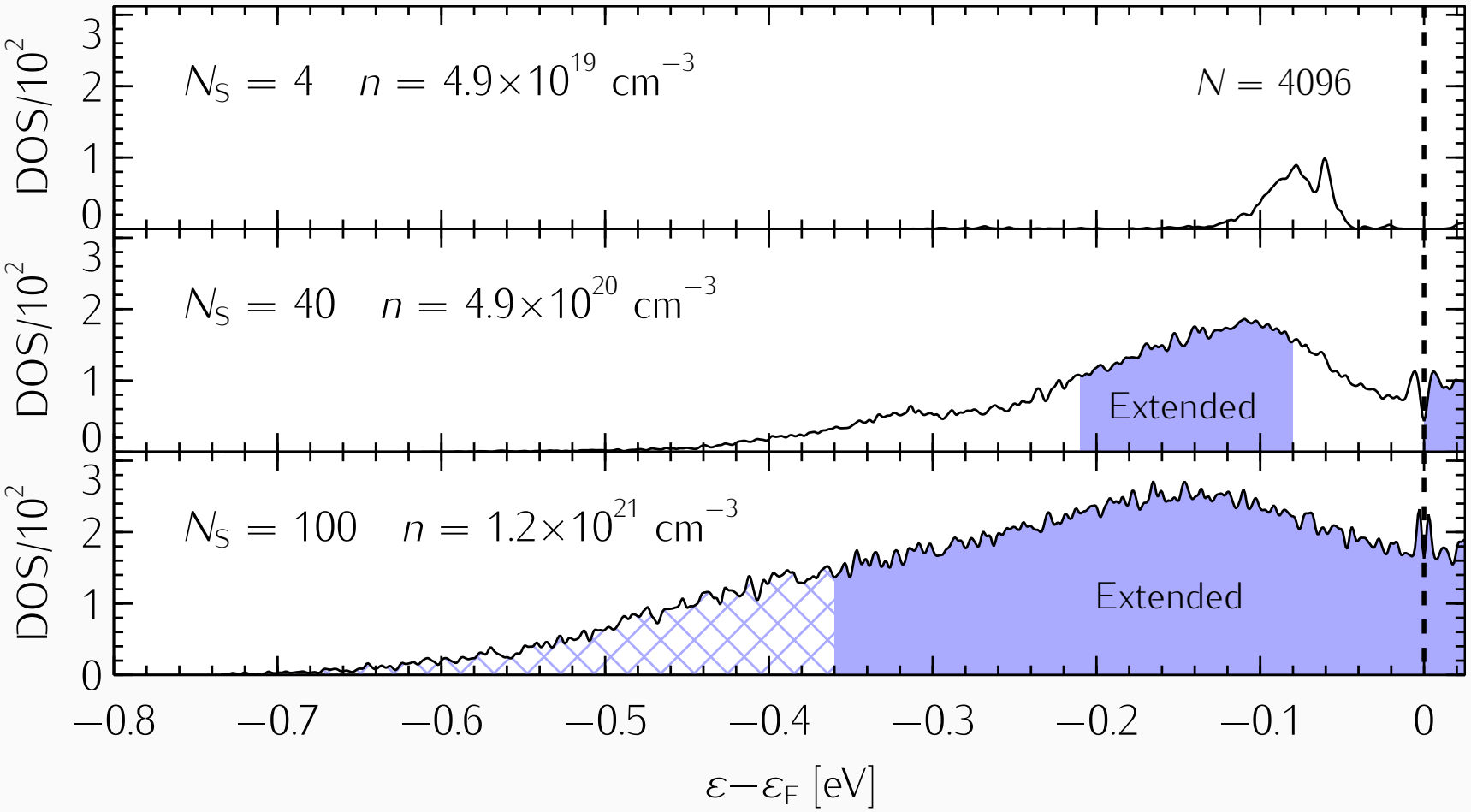


$$\mathcal{A}(\rho L^{1/\nu}) = \sum_i^{n_R} a_i (\rho L^{1/\nu})^i \qquad \rho = w + \sum_{i=2}^{m_\rho} b_i w^i \qquad w = \frac{n - n_c}{n_c} \quad (3)$$

[2] A. Rodriguez et al. *Phys. Rev. B* **2011**, 84, 134209.

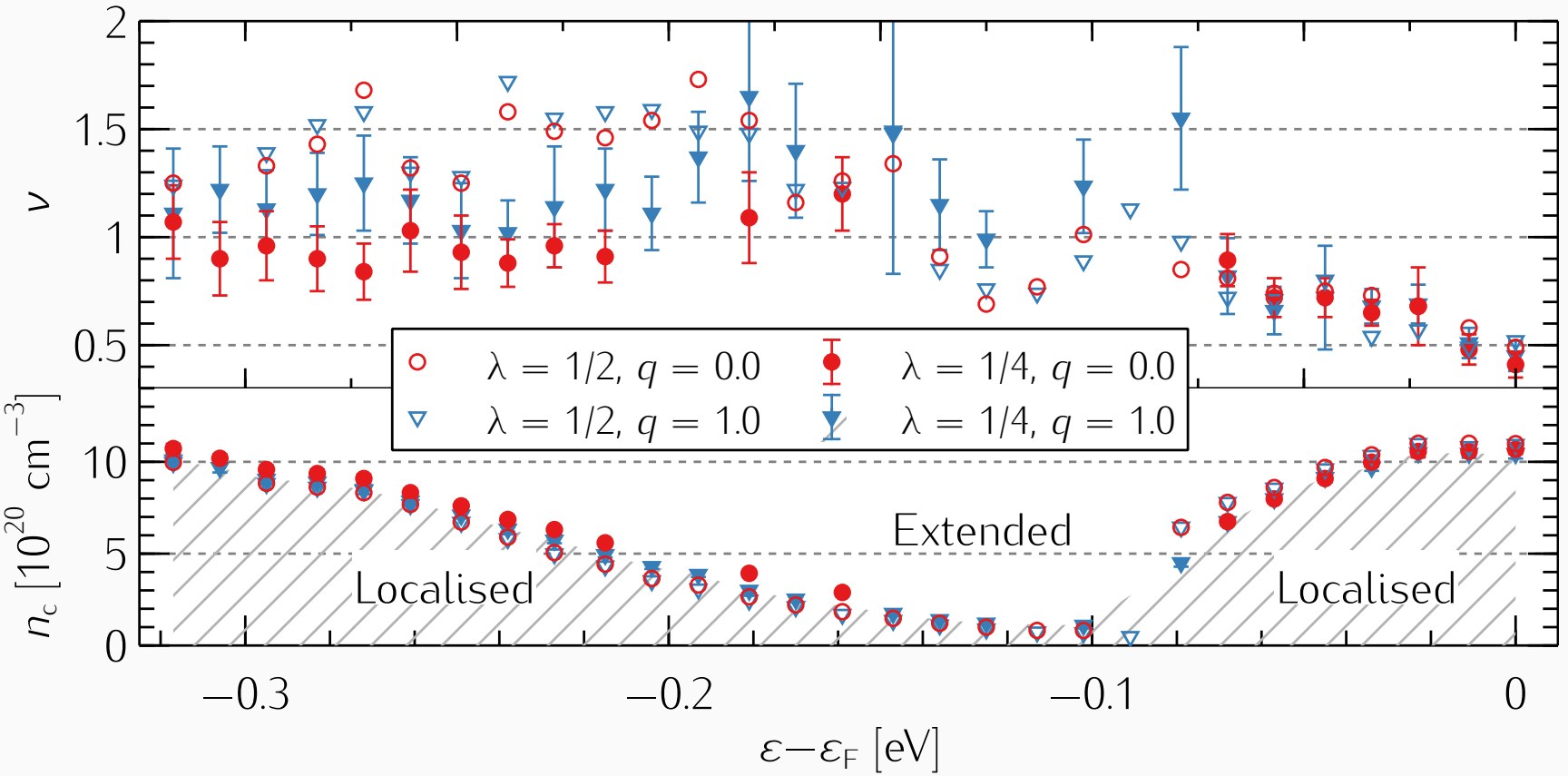
Results

DOS



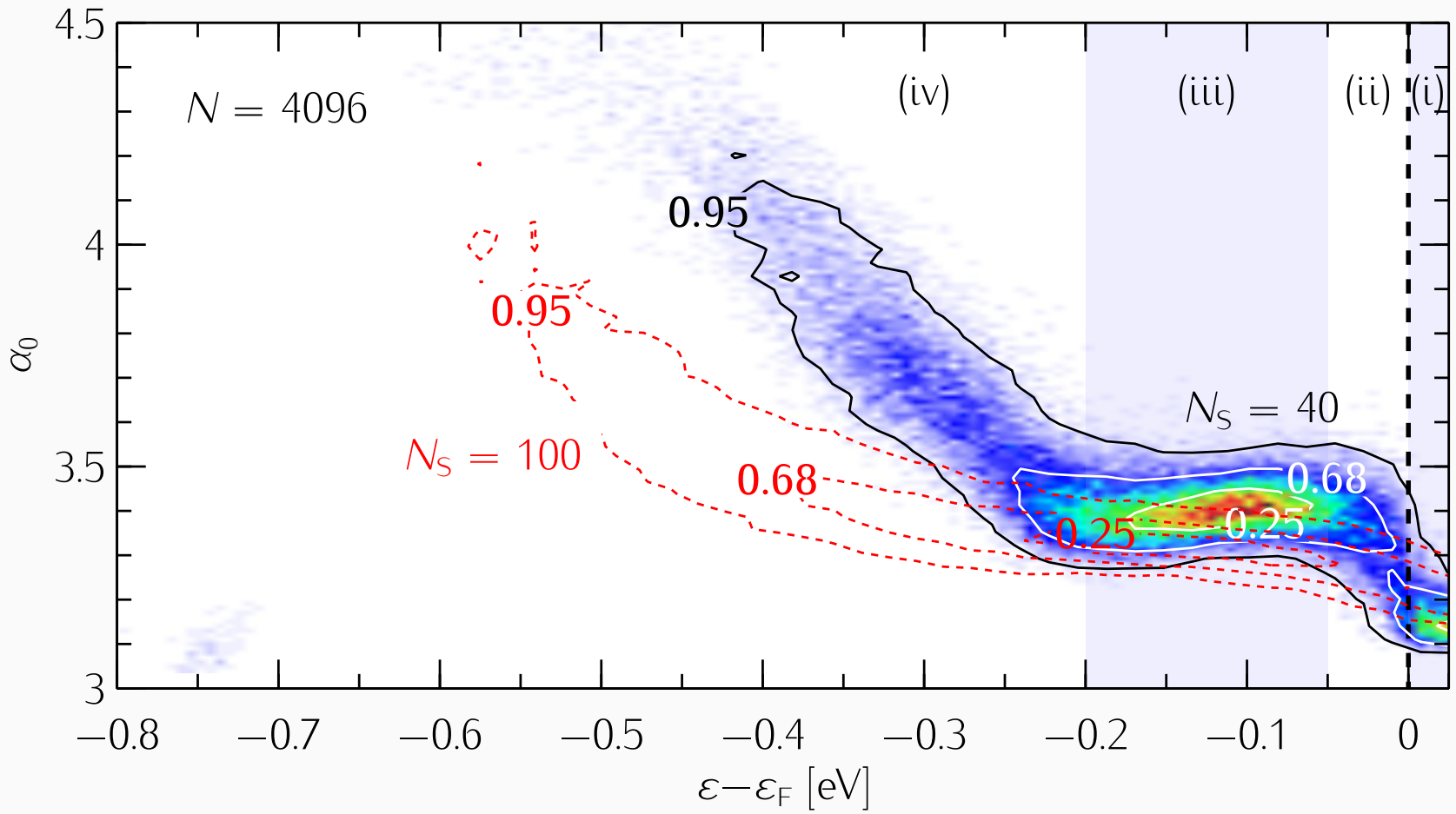
- *Asymmetric tail* extends towards the valence band.
- MIT: extended states and vanishing band gap.

Phase diagram



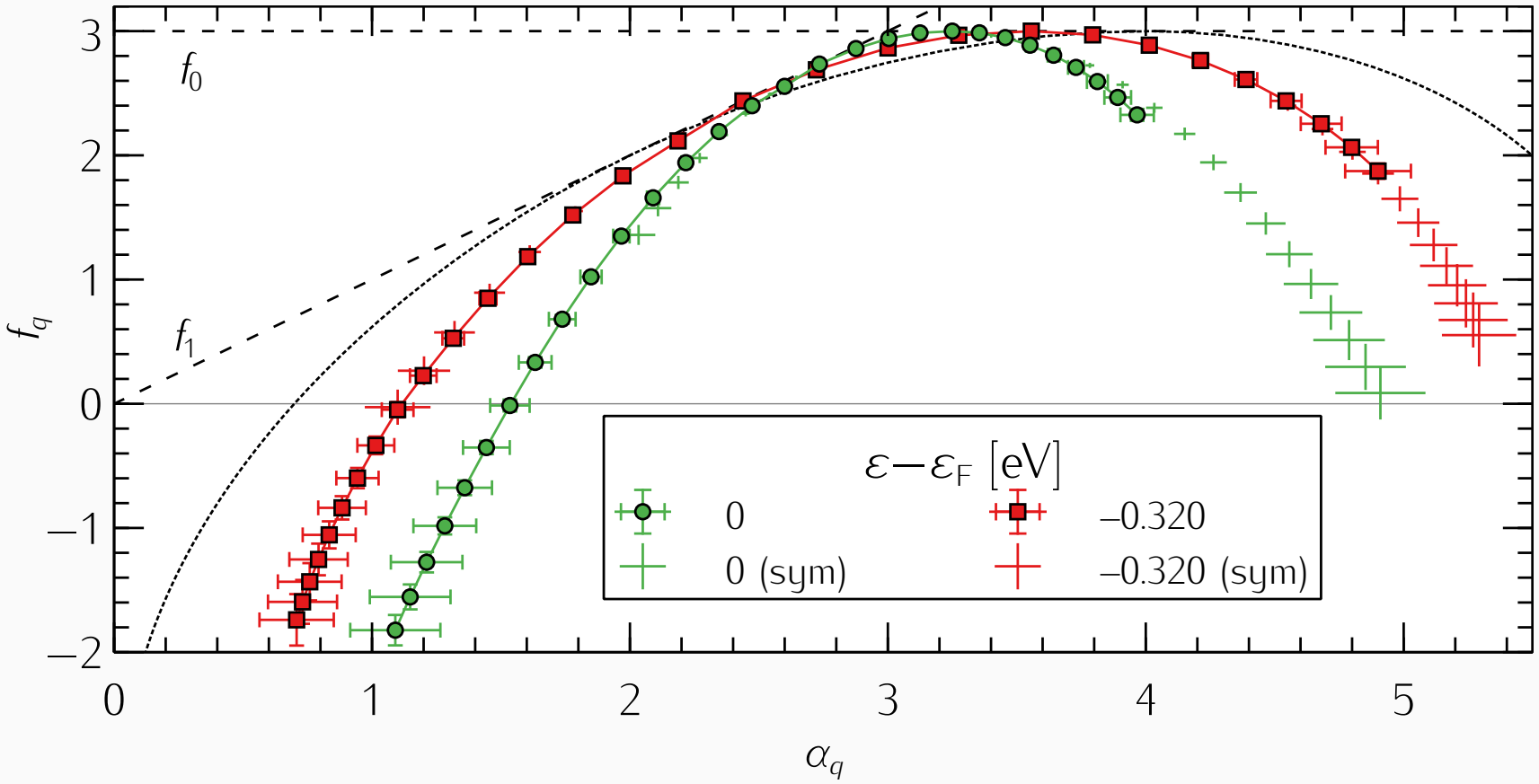
- Concave shape of n_c: delocalisation from band centre outwards.
- At the top of the band ν rises from 0.5 to 1 (experiments) and fluctuates between values 1 and 1.5 deeper in the band.

2D DOS and hybridisation



- Features: regimes distinguishable by localisation properties.
- Hybridised states (ii) connect the IB peak (iii) and the CB (i).

Multifractal spectrum (10410 Si + 230 S)



- Symmetry: $f(2d - \alpha) = f(\alpha) + d - \alpha$, with $d = 3$.
- "Quasi-metallic" behaviour (Anderson $2 + \epsilon$, PRBM).
- Behaviour is more pronounced at the Fermi energy.

Final thoughts

We have found that

1. near the Fermi energy states are more extended (hybridisation between IB and CB).
2. in the same energy range the ν varies from 0.5 to 1.

Are these observations connected? If yes, how?

Hypothesis: conductance scales as $\sigma \propto (n - n_c)^{\nu}$, where $n - n_c \ll 1$.

$$\text{Hybridisation} \Rightarrow \text{higher } \sigma \overset{?}{\Rightarrow} \text{reduced } \nu$$

Conclusions

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Take-home message

We use *ab initio* methods to simulate a doped semiconductor (Si:S).
We observe

- a MIT with increasing donor concentration;
- the hybridisation of impurity and conduction states near ε_F;
- the reduction of ν from 1-1.5 to 0.5 near ε_F.

Next questions:

- Connection between hybridisation and ν
- Improve estimates by going to larger L
- Study other semiconductors (compensated? 2D?)

More details:
E. G. Carnio, N. D. M. Hine, R. A. Römer, `arXiv:1710.01742`