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# Incoherent transport near the Mott transition

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## ABSTRACT

We examine the mechanism for the violation of the Mott-Ioffe-Regel (MIR) condition for the maximal metallic resistivity near the interaction-driven Mott transition. We find that the large resistivity appears due to the large scattering rate which destroys well-defined quasi-particles, while the Drude-like peak in the optical conductivity persists well beyond the MIR limit, similar as in the experiments on $\mathrm{VO_2}$. The disorder induces effective local carrier doping which moves the system away from the Mott insulator, increasing the conductivity, in agreement with the recent experiments on X-ray irradiated organic charge-transfer salts.

## Disordered Hubbard model

$$H = -\sum_{ij,\sigma} t_{i,j} d^\dagger_{i\sigma} d_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \varepsilon_i \sum_{i\sigma} n_{i\sigma}$$

- **DMFT approximation**
  Local Green's function $G_l(\tau-\tau) = -\langle T d_\sigma(\tau) d^\dagger_\sigma(\tau)\rangle_{S_{eff}}$ is obtained form the corresponding Anderson impurity model action [1]

$$\mathrm{S}^i_{eff} =$$
$$-\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma d^+_\sigma(\tau) \mathcal{G}^{-1}_{0i}(\tau-\tau') d_\sigma(\tau')$$
$$+U \int_0^\beta d\tau n_\uparrow(\tau) n_\downarrow(\tau),$$

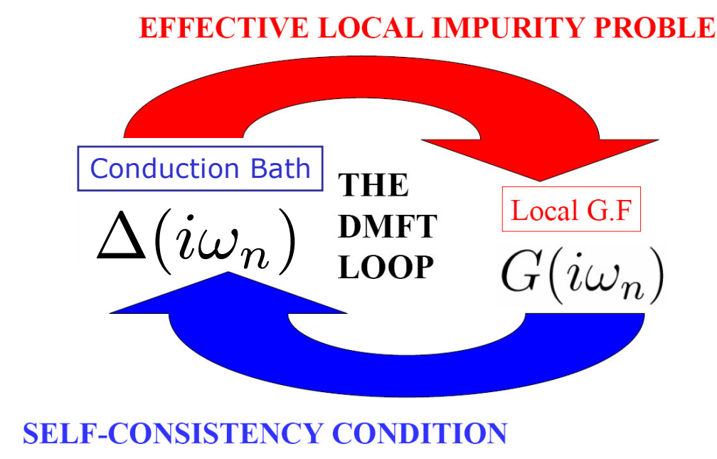
$$\mathcal{G}^{-1}_{0i}(i\omega_n) = i\omega_n + \mu - \varepsilon_i - \Delta(i\omega_n)$$

"Weiss field" random site energy conduction bath

Disorder averaging within CPA

$$G(i\omega_n) = \frac{1}{N} \sum_{i=1}^{N} G_i(i\omega_n)$$

DMFT self-consistency loop



$$G(i\omega_n) = \int d\varepsilon \frac{D(\varepsilon)}{\Delta(i\omega_n) + G(i\omega_n)^{-1} - \varepsilon}$$

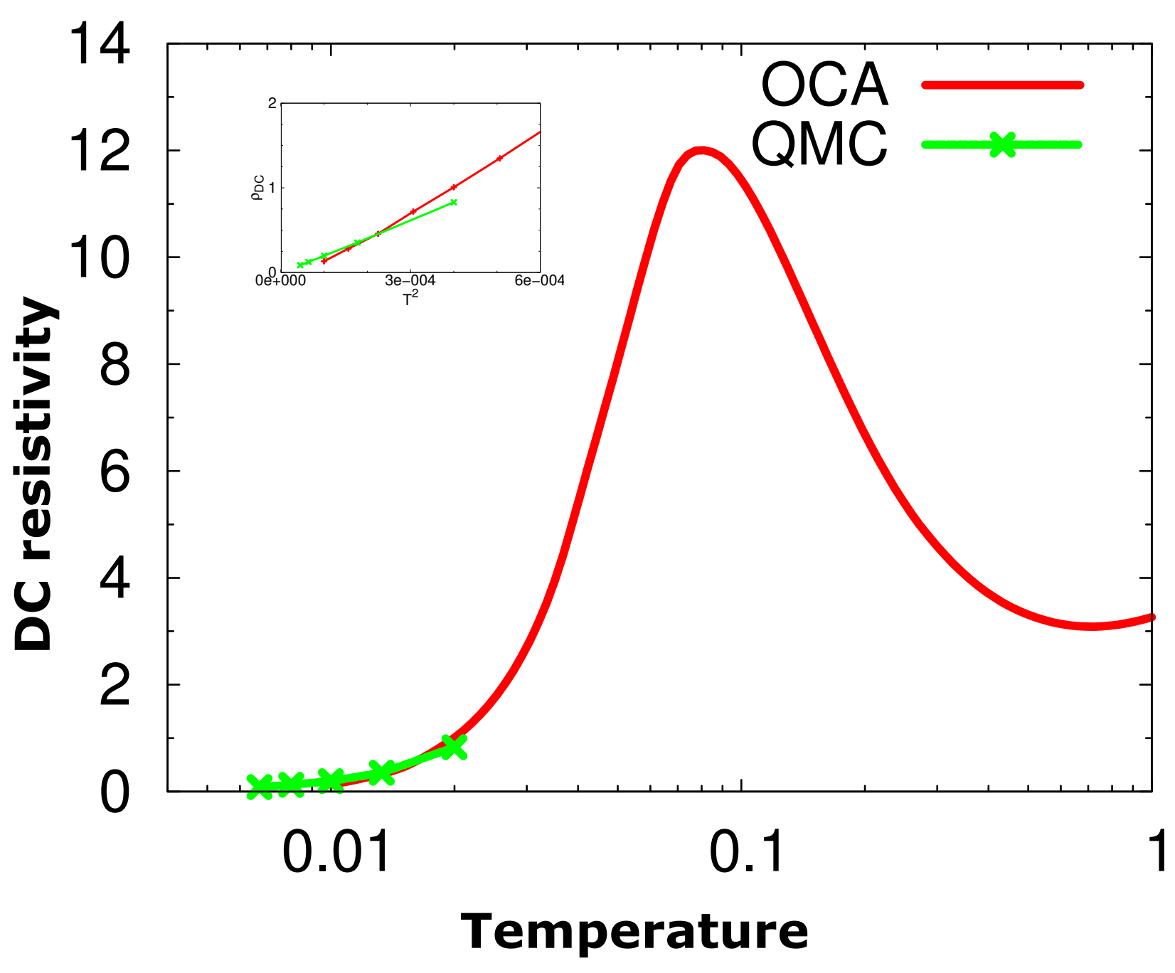
- **Kubo formula in DMFT approximation**

$$\sigma(i\omega) =$$
$$\frac{1}{\omega} \int_{-\infty}^{+\infty} d\epsilon \int_{-\infty}^{+\infty} d\nu \int_{-\infty}^{+\infty} d\nu' D(\epsilon) \rho(\epsilon,\nu) \rho(\epsilon,\nu') \frac{f(\nu)-f(\nu')}{\nu-\nu'+i\omega}$$

DC resistivity: $\rho_{DC} = \sigma^{-1}(\omega \to 0)$

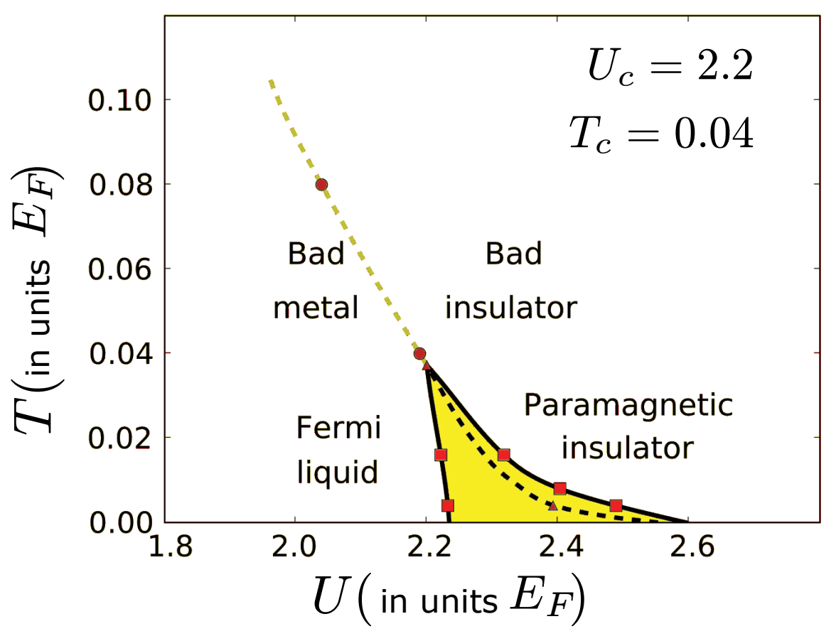
## Impurity solvers

Anderson impurity model is solved using One-Crossing Approximation (OCA) (generalized NCA) [2,3], and the results are cross-checked with numerically exact Continues Time Quantum Monte Carlo (CTQMC) [4] impurity solver.

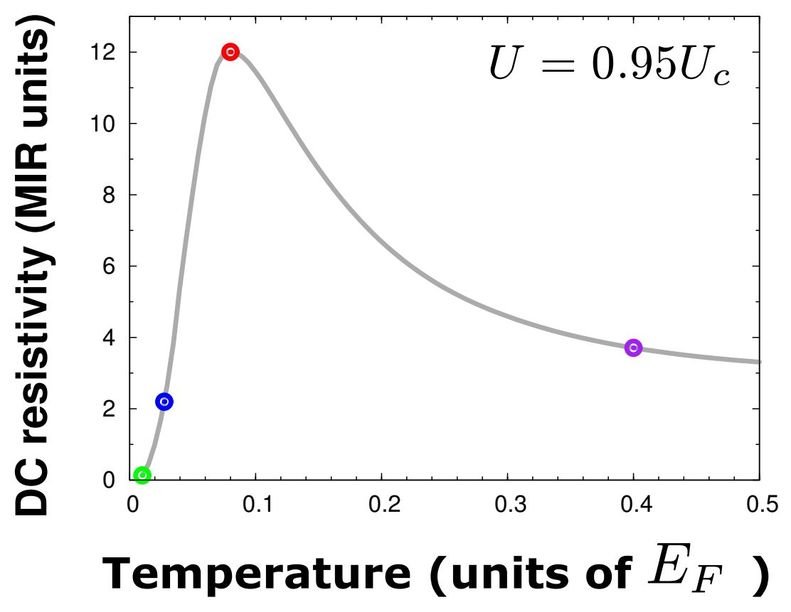


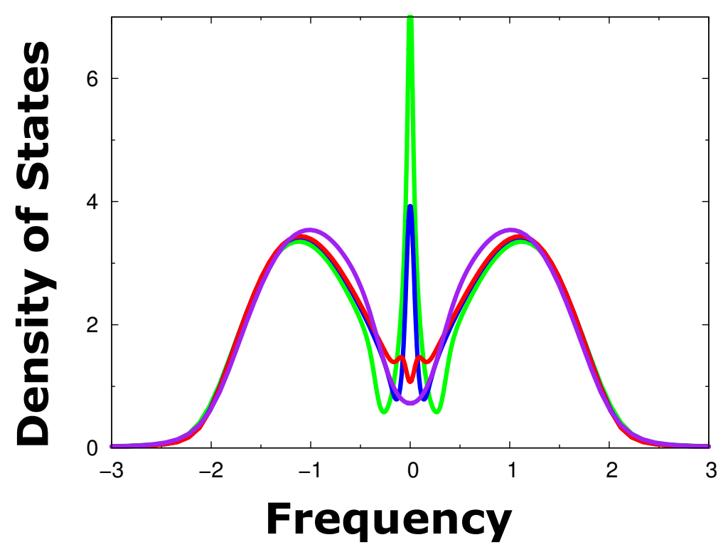
## Violation of the MIR condition

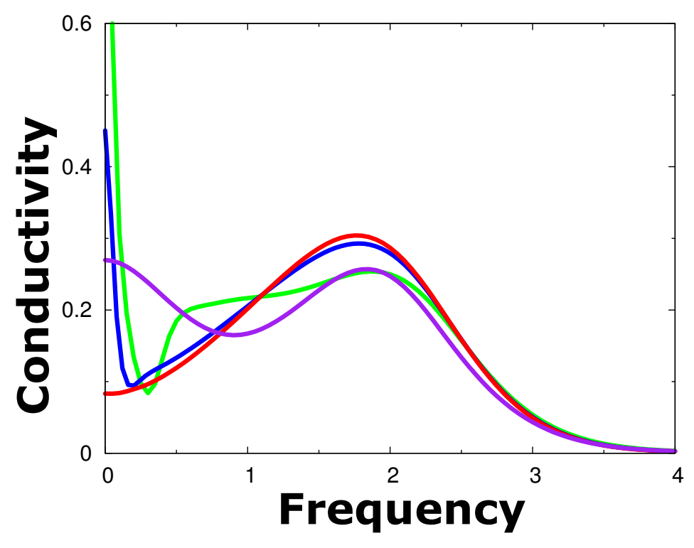
- **Mott-Ioffe-Regel limit** is the maximal metallic resistivity, $\rho_{MIR}$, which is reached when the mean free path of the electron becomes comparable to the lattice spacing [5]
$$l \sim a \Leftrightarrow E_F\tau \sim 1.$$
  According to semi-classical arguments, resistivity cannot be larger than MIR limit.
- **Mott metal-insulator transition**



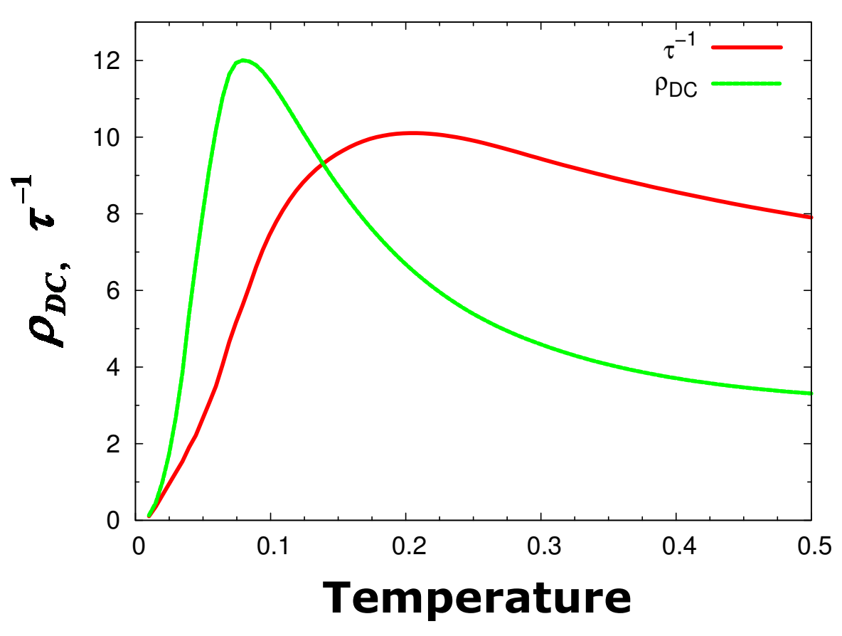
- **Results near the critical point**
  -Fermi liquid at low temperatures.
  -Drude-like peak persists well above the MIR limit.
  -Maximal resistivity is an order of magnitude larger than $\rho_{MIR}$.





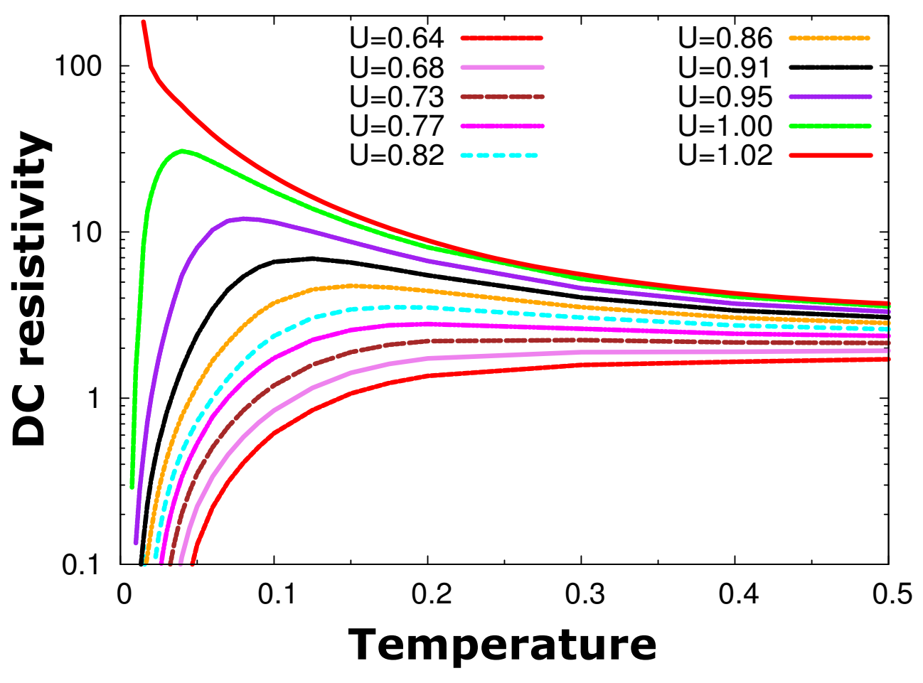


- Large **scattering rate**, $\tau^{-1} = -\frac{1}{2} Im\Sigma(0^+)$, gives the main contribution to the resistivity temperature dependence, and causes the violation of the MIR condition. Above the MIR limit, $\tau^{-1} > E_F$ , and therefore, well-defined quasi-particles do not exist. Similar conclusions are obtained from experiments on $\mathrm{VO_2}$ [6], and $\kappa$-organics [7].



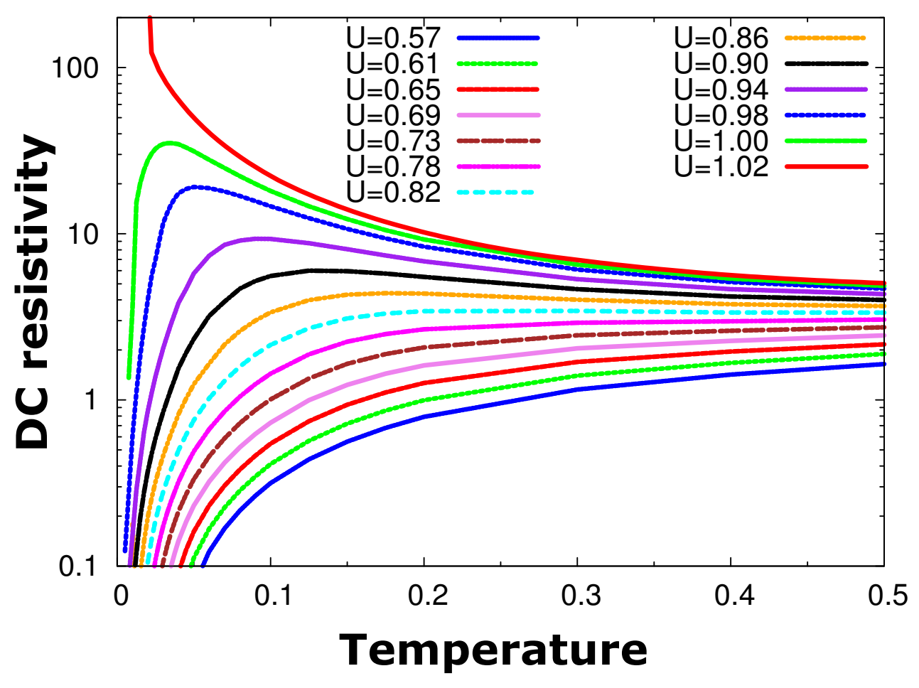
## Effects of disorder

- **Disorder** effectively increases the bandwidth, and the critical interaction $U_c$. Maximal value of $\rho_{DC}$, and the critical temperature do not change appreciably with disorder.



**Pure case**

$U$ in units $U^0_c$

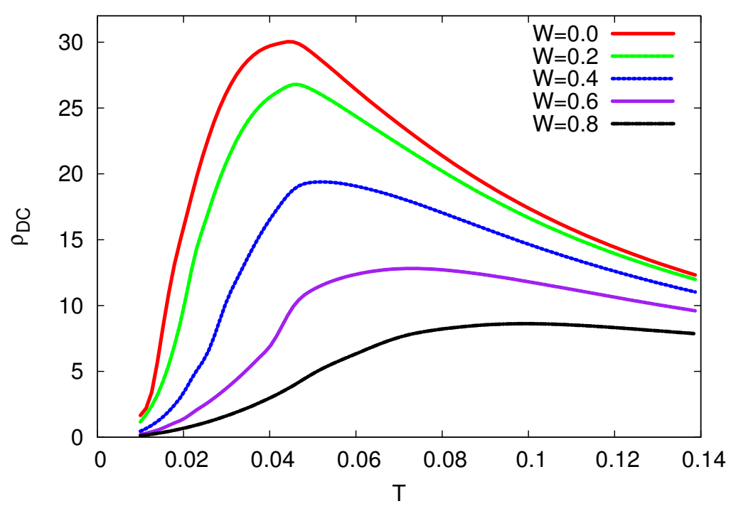


**Disordered case**

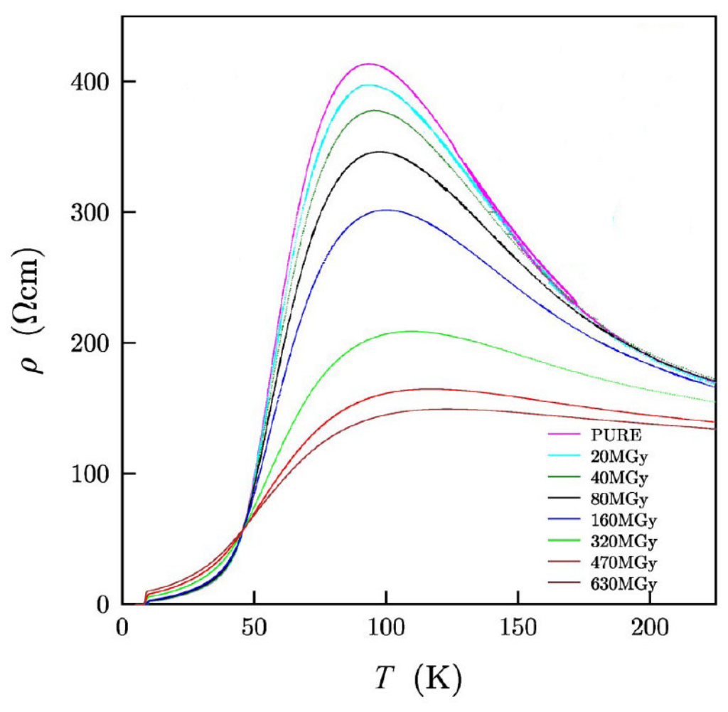
Uniformly distributed disorder in $(-W/2, W/2)$, $U$ in units $U_c(W)$.

Here $U^0_c = 2.2, W = 1$, $U_c = 2.45$. Increase in $U_c$ with $W$ agrees with earlier estimates [8].

- **Resistivity for fixed U**

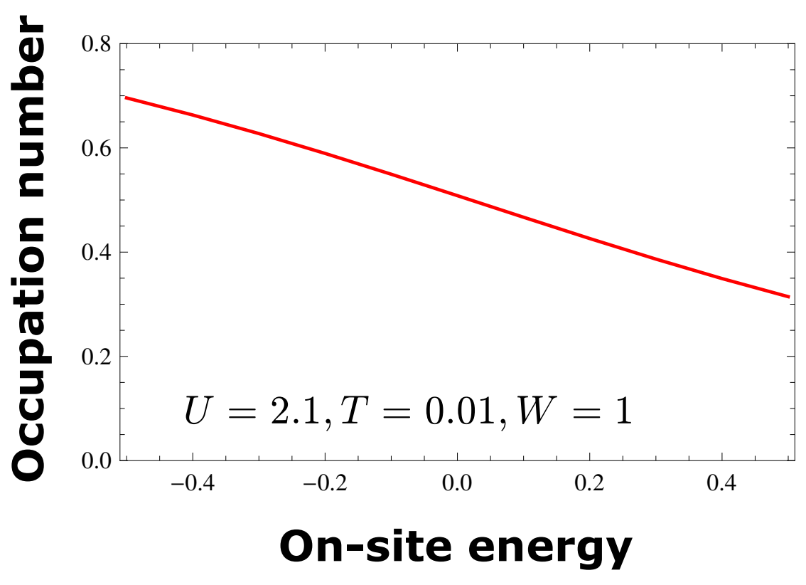


$U$ is fixed to $U^0_c$, disorder is varied



Experiments on X-ray irradiated $\kappa\text{-}(\mathrm{BEDT\text{-}TTF})_2\mathrm{Cu(SCN)}_2$ [9]

- **Effective local carrier doping by disorder**
  Random site energies change the local occupation number from half-filling, reducing the correlation effects and decreasing the resistivity. Similar physical picture is proposed as the explanation of the experiments on $\kappa$-organics [10].



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