

Nadprzewodnictwo wysokotemperaturowe oraz inne stany o złamanej symetrii w układach silnie skorelowanych elektronów

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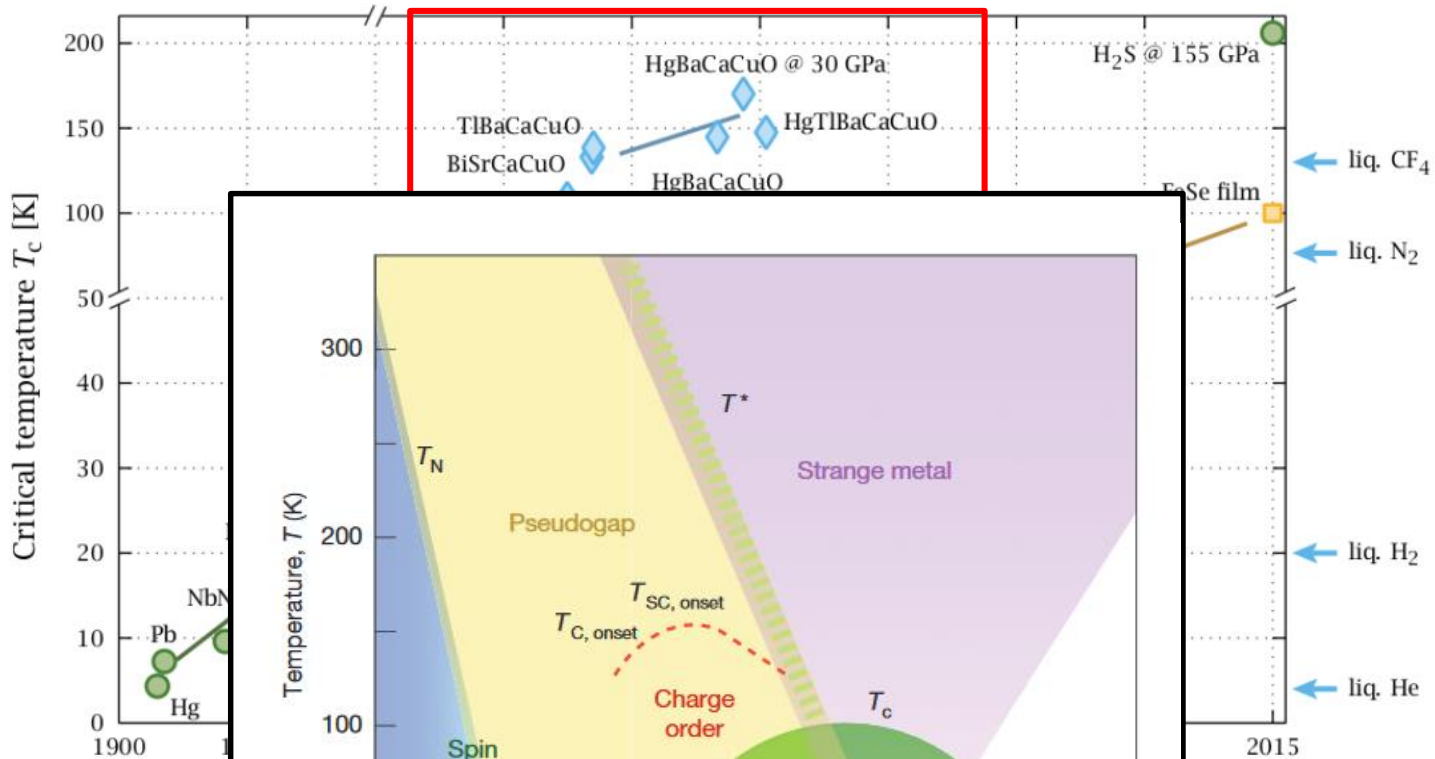
²*Instytut Fizyki im. Mariana Smoluchowskiego, Uniwersytet Jagielloński, Kraków*

Nadprzewodnictwo wysokotemperaturowe oraz inne stany o złamanej symetrii w układach silnie skorelowanych elektronów

- [1] **M. Zegrodnik**, A. Biborski, M. Fidrysiak, J. Spałek. "Superconductivity in the three-band model of cuprates: Variational wave function study and relation to the single-band case". *Phys. Rev. B* **99**, 104511 (2019)
- [2] **M. Zegrodnik**, J. Spałek. "Incorporation of charge- and pair-density-wave states into the one-band model of d-wave superconductivity". *Phys. Rev. B* **98**, 155144 (2018)
- [3] **M. Zegrodnik**, J. Spałek. "Stability of the coexistent superconducting-nematic phase under the presence of intersite interactions". *New J. Phys.* **20**, 063015 (2018)
- [4] **M. Zegrodnik**, J. Spałek. "Effect of interlayer processes on the superconducting state within the $t - J - U$ model: Full Gutzwiller wave-function solution and relation to experiment". *Phys. Rev. B* **95**, 024507 (2017)
- [5] **M. Zegrodnik**, J. Spałek. "Universal properties of high-temperature superconductors from real-space pairing: Role of correlated hopping and intersite Coulomb interaction within the $t - J - U$ model". *Phys. Rev. B* **96**, 054511 (2017)
- [6] J. Spałek, **M. Zegrodnik**, J. Kaczmarczyk. "Universal properties of high-temperature superconductors from real-space pairing: $t - J - U$ model and its quantitative comparison with experiment". *Phys. Rev. B* **95**, 024506 (2017)
- [7] M. Abram, **M. Zegrodnik**, J. Spałek. "Antiferromagnetism, charge density wave, and d-wave superconductivity in the extended $t - J - U$ model: role of intersite Coulomb interaction and a critical overview of renormalized mean field theory". *J. Phys. Condens. Matter* **29**, 365602 (2017)
- [8] **M. Zegrodnik**, J. Spałek. "Spontaneous Appearance of the Spin-Triplet Fulde-Ferrell-Larkin-Ovchinnikov Phase in a Two-Band model: Possible Application to $\text{LaFeAsO}_{1-x}\text{F}_x$ ". *J. Supercond. Nov. Magn.* **28**, 1155 (2015)
- [9] **M. Zegrodnik**, J. Spałek. "Spontaneous appearance of nonzero-momentum Cooper pairing: Possible application to the iron-pnictides". *Phys. Rev. B* **90**, 174507 (2014)

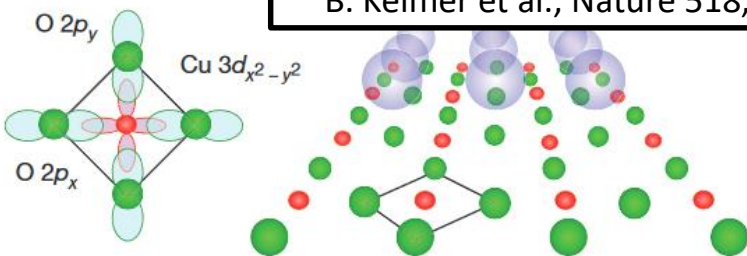
Plan prezentacji

- **Nadprzewodniki wysokotemperaturowe na bazie miedzi**
- **Opis teoretyczny płaszczyzn miedziowo-tlenowych**
- **Podstawowe charakterystyki stanu nadprzewodzącego w ujęciu jednopasmowym**
- **Stany z modulacją ładunkową oraz modulacją gęstości par Coopera**
- **Wpływ tlenowych stopni swobody na nadprzewodnictwo – porównanie modeli jedno- oraz trój-pasmowych**
- **Podsumowanie**

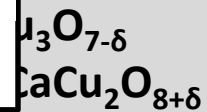


B. Keimer et al., Nature 518, 179 (2015)

- O
- Cu
- Ba/Ca



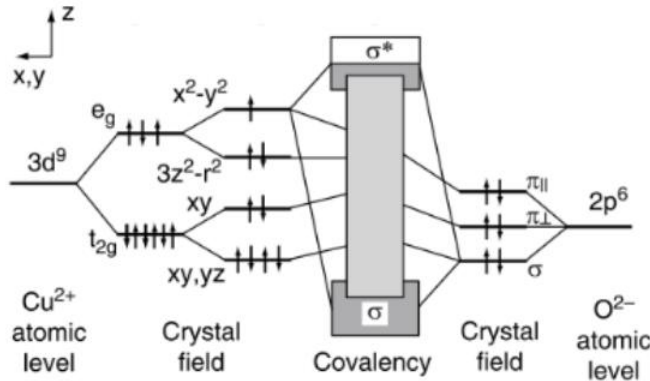
owanie:



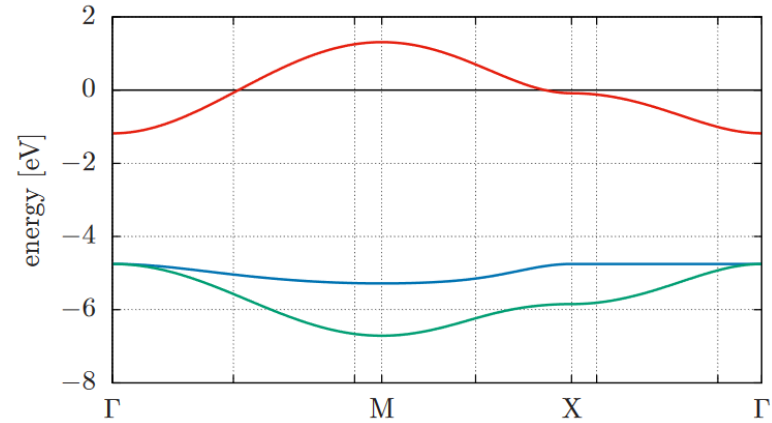
- $\text{HgBa}_2\text{CuO}_{4+\delta}$
- $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$

Nadprzewodniki na bazie miedzi

Rozszczepienie poziomów energetycznych:



Model trój-pasmowy (model d-p):



Efektywny model jedno-pasmowy:

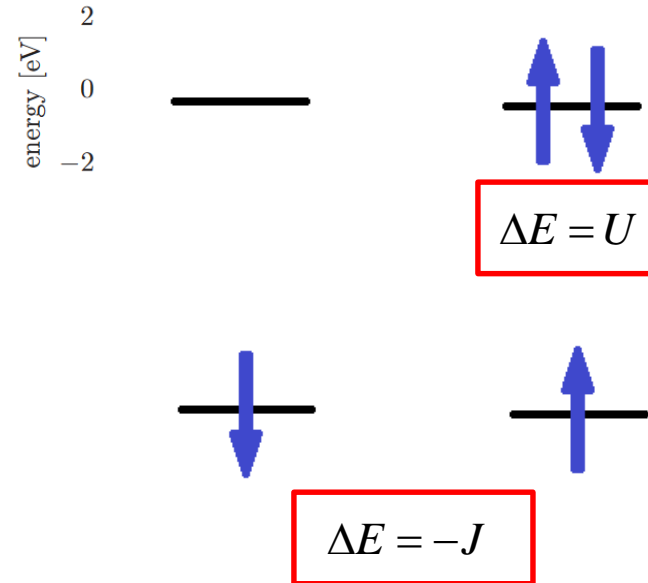
$$\hat{H} = t \sum_{\langle ij \rangle \sigma} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + t' \sum_{\langle\langle ij \rangle\rangle \sigma} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

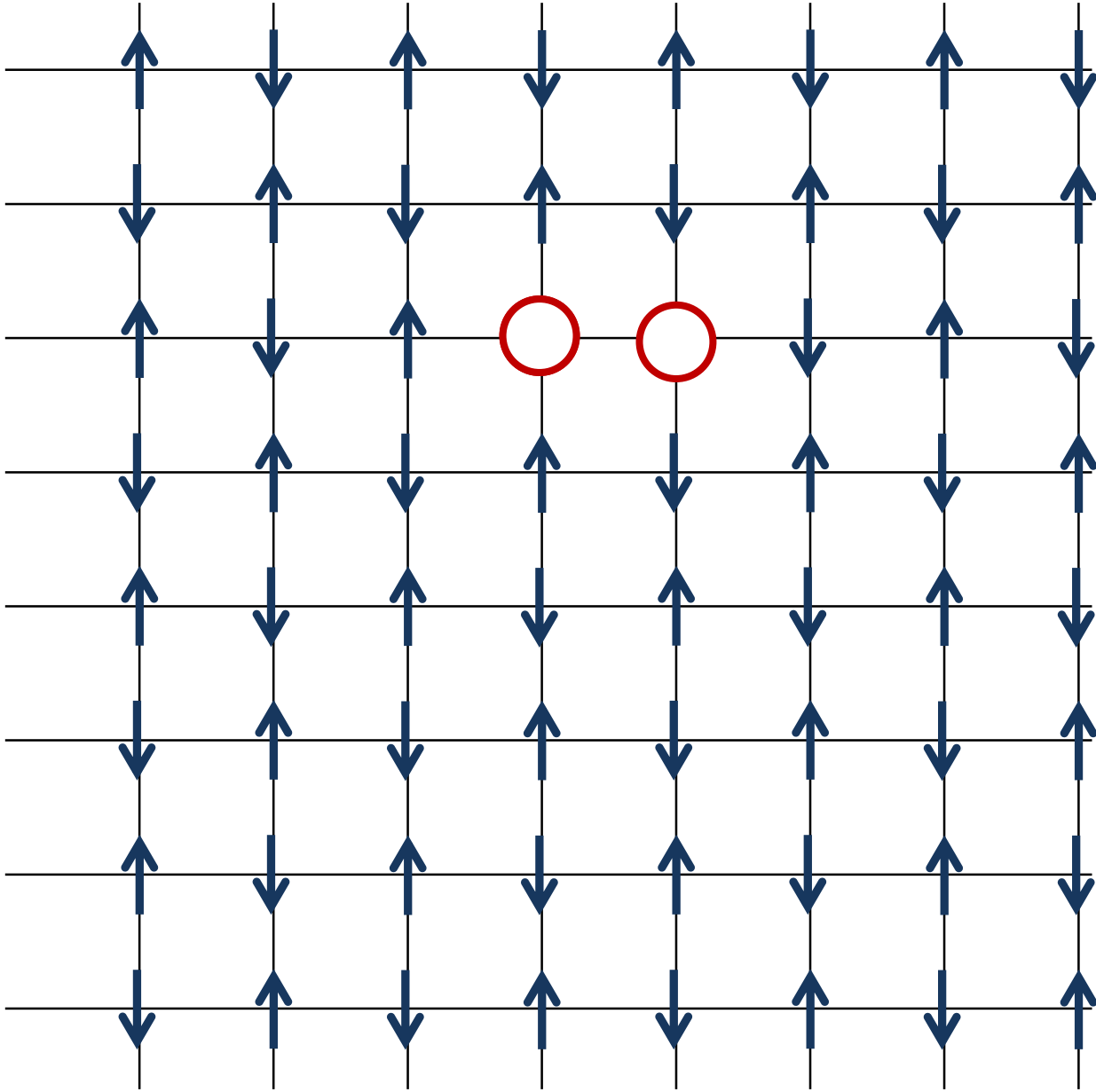
$$t = -0.35 \text{ eV}, t' = 0.0875 \text{ eV}, U = 6-8 \text{ eV}$$

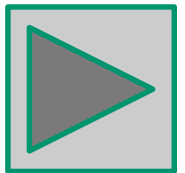
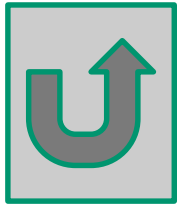
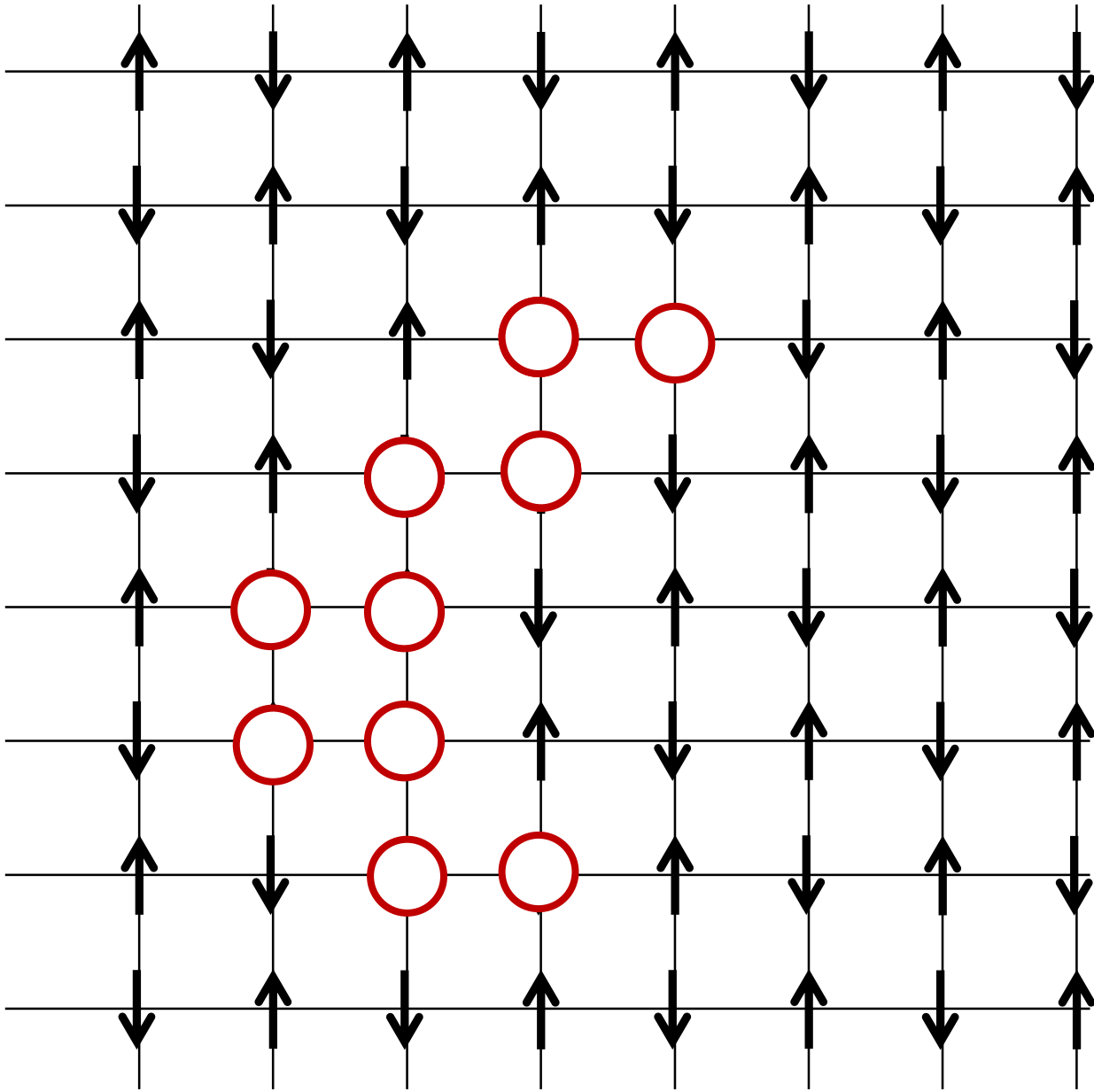
Model t - J ($U \rightarrow \infty$):

$$\hat{H} = t \sum_{\langle ij \rangle \sigma} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + t' \sum_{\langle\langle ij \rangle\rangle \sigma} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + J \sum_{\langle ij \rangle} \hat{S}_i \hat{S}_j$$

$$t = -0.35 \text{ eV}, t' = 0.0875 \text{ eV}$$

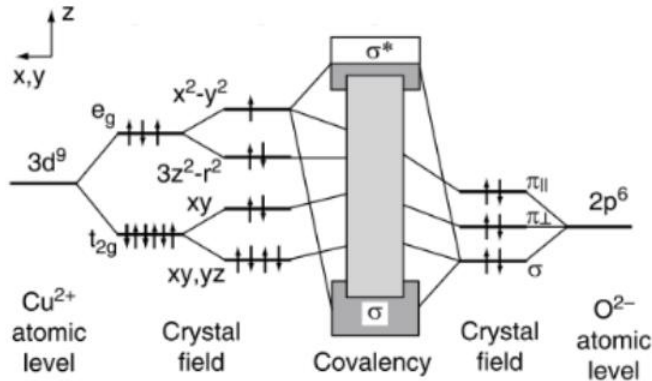




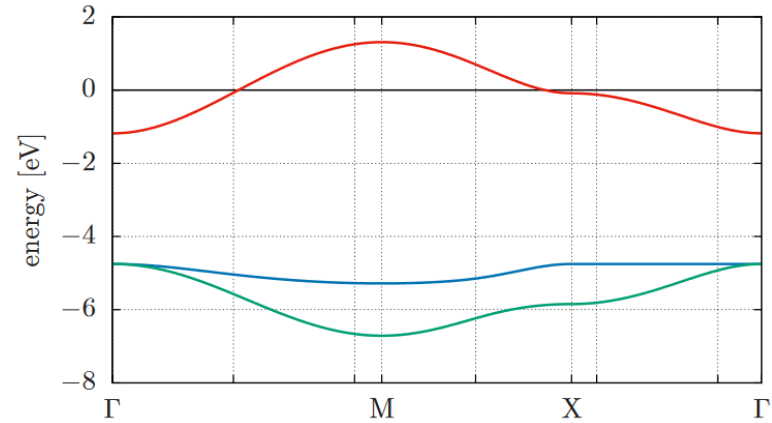


Nadprzewodniki na bazie miedzi

Rozszczepienie poziomów energetycznych:



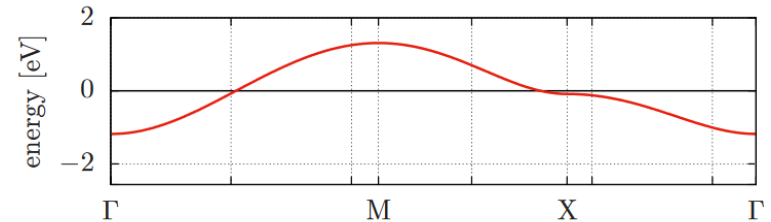
Model trój-pasmowy (model d-p):



Efektywny model jedno-pasmowy:

$$\hat{H} = \sum_{\langle ij \rangle \sigma} t \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + \sum_{\langle\langle ij \rangle\rangle \sigma} t' \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$t = -0.35 \text{ eV}, t' = 0.0875 \text{ eV}, U = 6-8 \text{ eV}$$



Model t-J-U:

$$\hat{H} = \sum_{\langle ij \rangle \sigma} t \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + \sum_{\langle\langle ij \rangle\rangle \sigma} t' \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + J \sum_{\langle ij \rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

$$t = -0.35 \text{ eV}, t' = 0.0875 \text{ eV}, J = 0.1 \text{ eV}, U = 6-8 \text{ eV}$$

$$\hat{H} = t \sum_{\langle ij \rangle \sigma} \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} + J \sum_{\langle\langle ij \rangle\rangle} \hat{\mathbf{S}}_i \cdot \hat{\mathbf{S}}_j + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}$$

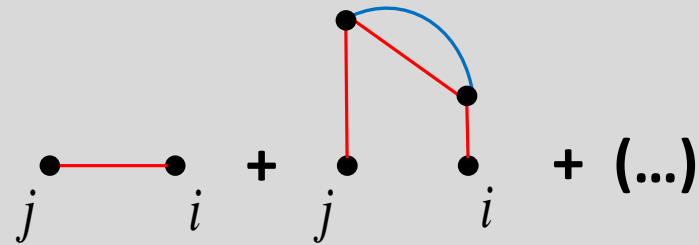
$$|\Psi_G\rangle = \hat{P}|\Psi_0\rangle = \prod_i \sum_{\Gamma} \lambda_{\Gamma} |\Gamma\rangle_{ii} \langle \Gamma | \Psi_0 \rangle, \quad \{|\Gamma\rangle_i\} = \{|\phi\rangle_i, |\uparrow\rangle_i, |\downarrow\rangle_i, |\uparrow\downarrow\rangle_i\}$$

RMFT



$$\langle \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} \rangle_G = q \langle \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} \rangle_0$$

DE-GWF



$$\langle \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} \rangle_G = \sum_{k=0}^{\infty} \frac{x^k}{k!} \sum_{l_1, \dots, l_k} \langle \tilde{c}_{i\sigma}^+ \tilde{c}_{j\sigma} \hat{d}_{l_1}^{HF} \hat{d}_{l_2}^{HF} \dots \hat{d}_{l_k}^{HF} \rangle_0$$

$$\hat{P}_i^2 = 1 + x \hat{d}_i^{HF}$$

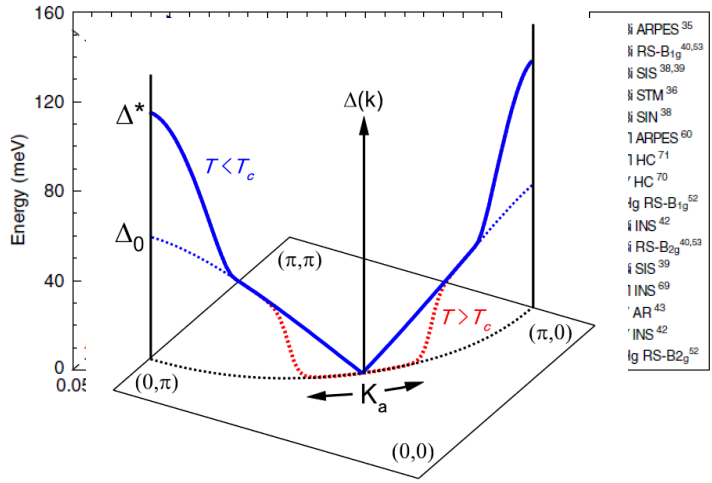
$$\hat{d}_i^{HF} = \hat{n}_{i\uparrow}^{HF} \hat{n}_{i\downarrow}^{HF}, \quad \hat{n}_{i\sigma}^{HF} = \hat{n}_{i\sigma} - \langle \hat{n}_{i\sigma} \rangle_0$$

$$E_G = \frac{\langle \Psi_G | \hat{H} | \Psi_G \rangle}{\langle \Psi_G | \Psi_G \rangle} = F(P_{ij}, S_{ij}, x)$$

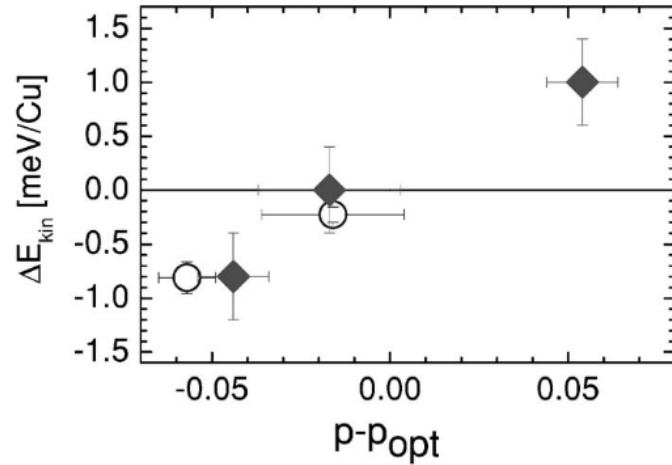
$$P_{ij} = \langle \Psi_0 | \hat{c}_{i\sigma}^+ \hat{c}_{j\sigma} | \Psi_0 \rangle, \quad S_{ij} = \langle \Psi_0 | \hat{c}_{i\uparrow}^+ \hat{c}_{j\downarrow}^+ | \Psi_0 \rangle$$

Fundamentalne charakterystyki stanu nadprzewodzącego w miedzianach

S. Yashni et al., *Rep. Prog. Phys.* **71** (2008) 062501



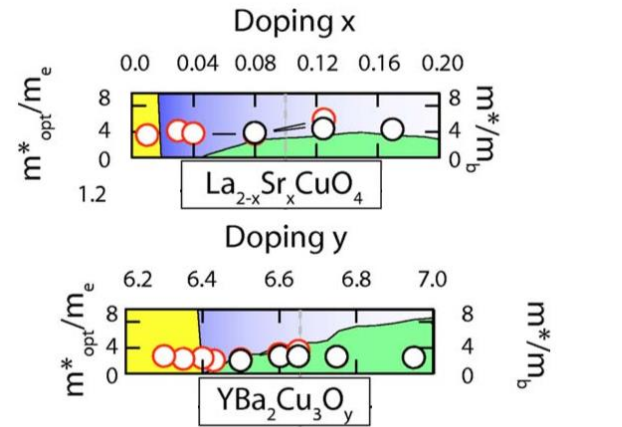
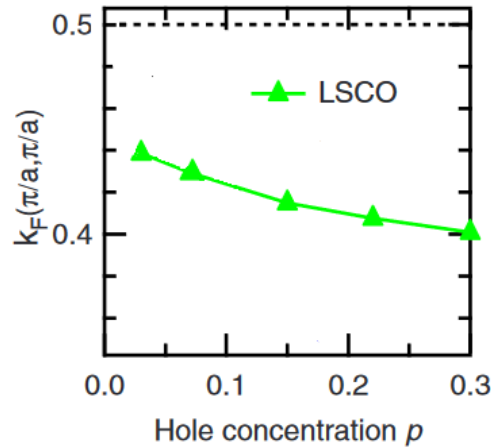
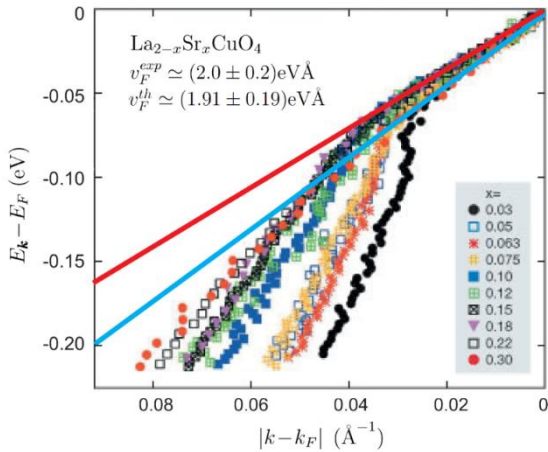
G. Deutscher et al., *PRB* **72**, 09250 (2005)



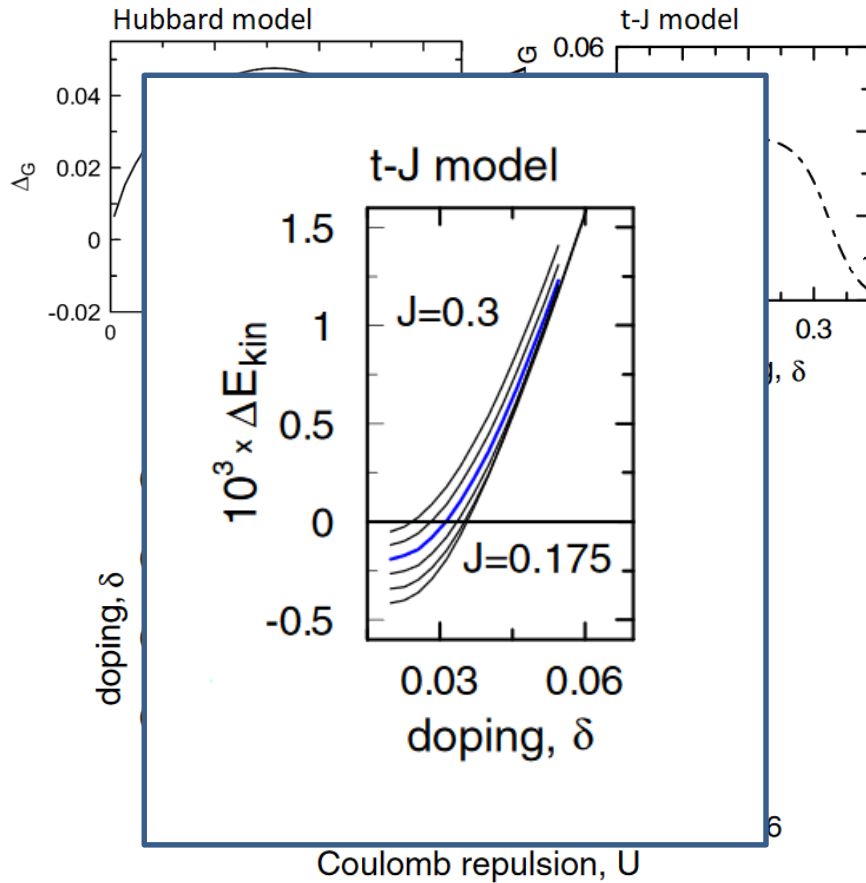
XJ. Zhou et al., *Nature* **423**, 398 (2003)

M. Hashimoto et al., *PRB* **094516** (2008)

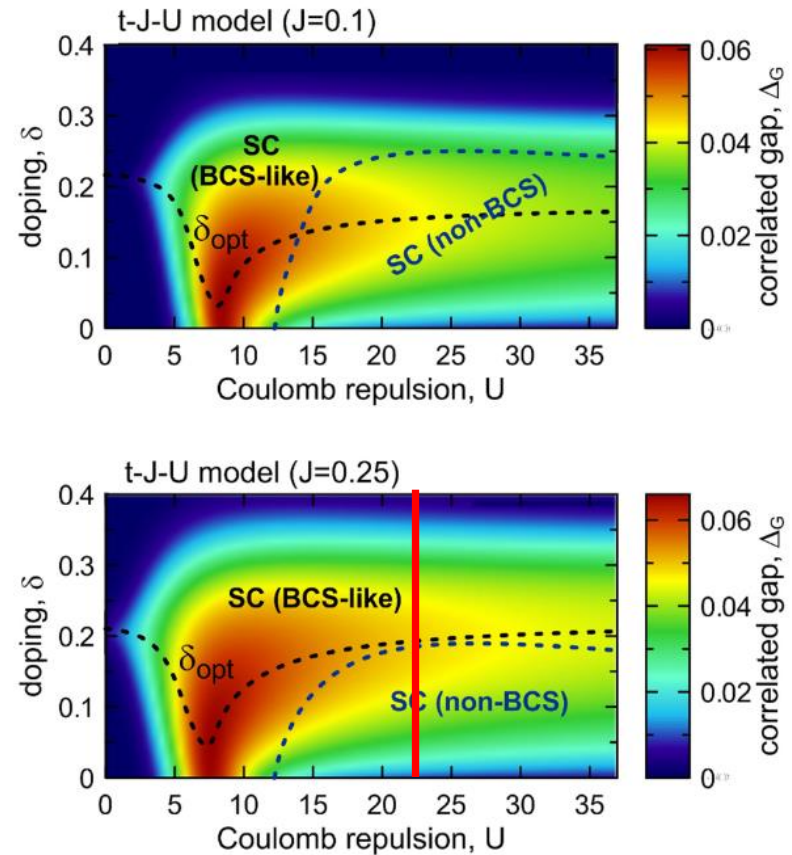
W. J. Padilla et al., *PRB* **72**, 060511 (2005)



modele Hubbarda, t-J, oraz t-J-U



$$\Delta_G = \langle \psi_G | \hat{a}_{i\uparrow}^+ \hat{a}_{j\downarrow}^+ | \psi_G \rangle / \langle \psi_G | \psi_G \rangle$$



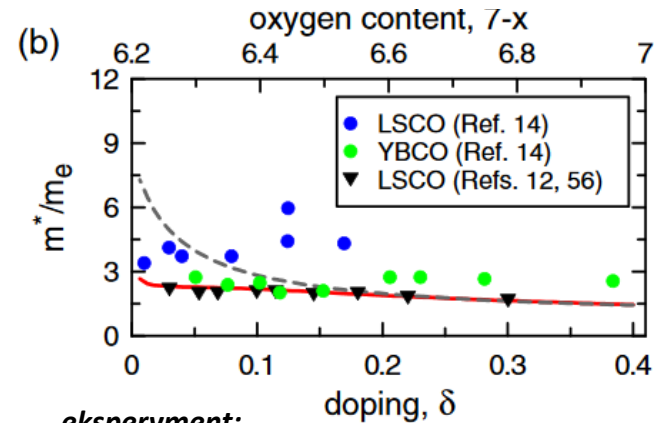
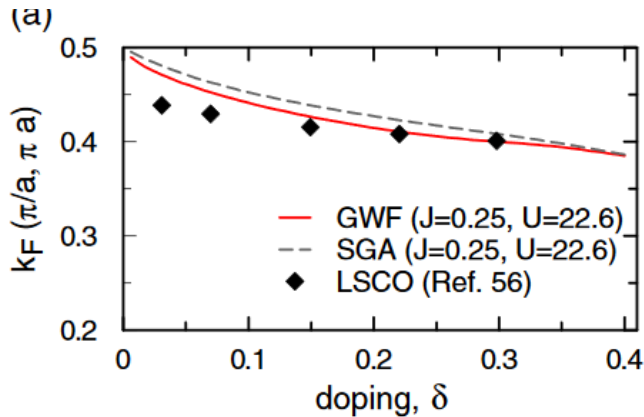
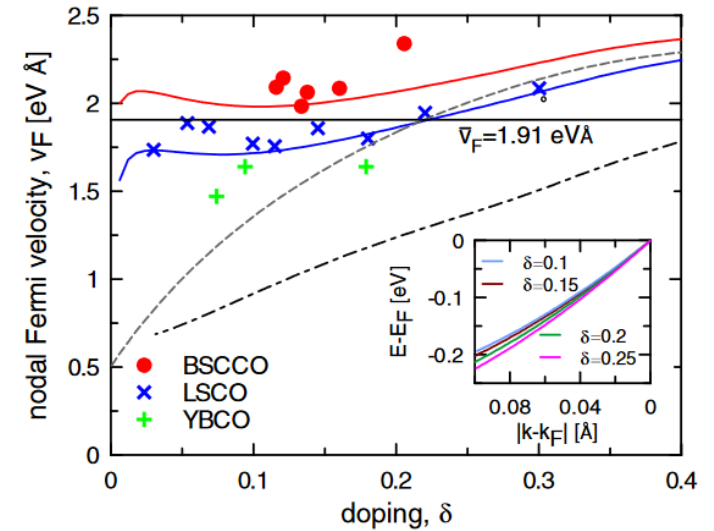
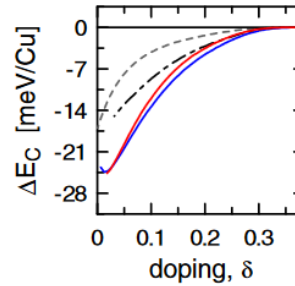
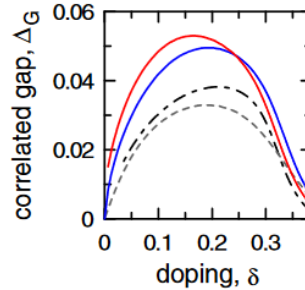
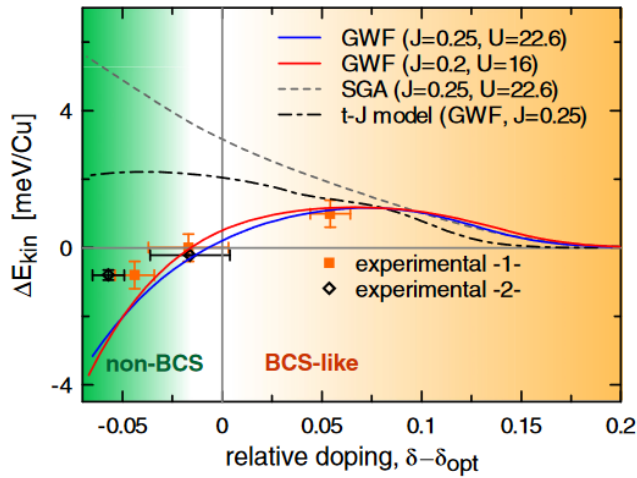
BCS - like :

$$\Delta E_{kin} = E_{kin}^{SC} - E_{kin}^{PM} > 0$$

non - BCS :

$$\Delta E_{kin} = E_{kin}^{SC} - E_{kin}^{PM} < 0$$

model t-J-U porównanie ilościowe z eksperymentem



teoria:

J. Spátek, MZ, and J. Kaczmarczyk, *Phys. Rev. B* 95, 024506 (2017)

MZ and J. Spátek, *Phys. Rev. B* 95, 024507 (2017)

MZ and J. Spátek, *Phys. Rev. B* 96, 054511 (2017)

eksperyment:

G. Deutscher et al., *Phys. Rev. B* 72, 092504 (2005);

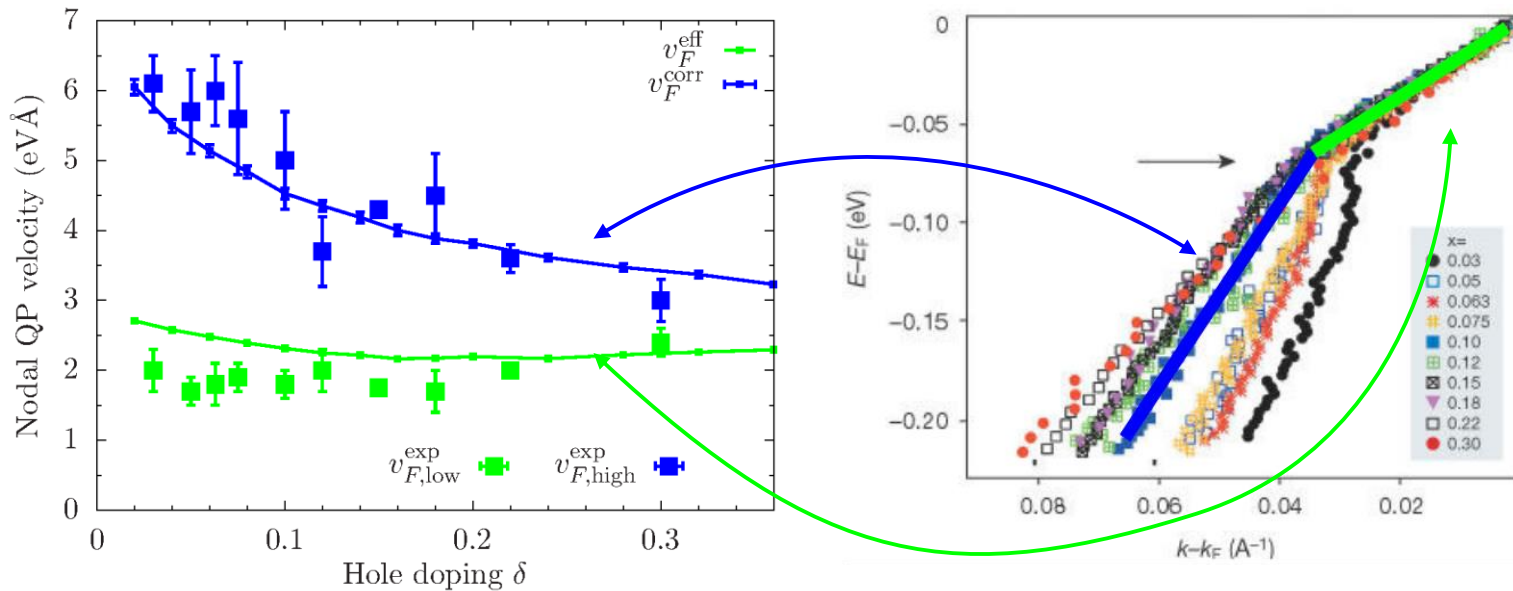
F. Carbonne et al., *Phys. Rev. B* 74, 064510 (2006);

H.J.A. Molegraaf et al., *Science* 295, 2239 (2002);

A.A. Kordyuk et al., *Phys. Rev. B* 71, 214513 (2005);

S.V. Borisenko et al., *Phys. Rev. Lett.* 96, 117004 (2006)

dwie prędkości Fermiego: porównanie ilościowe z eksperymentem



Teoria (k-DE-GWF):

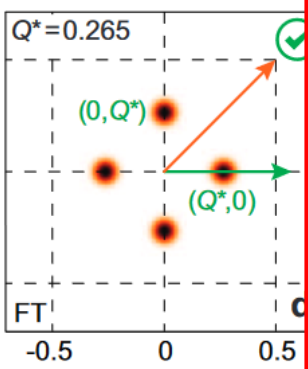
M. Fidrysiak, MZ, J. Spałek, *J. Phys. Condens. Matter* 30, 475602 (2018)

Eksperyment:

X. J. Zhou et al., *Nature* 423, 398 (2003); Matsuyama et al., *Phys. Rev. B* 95, 165435 (2017).

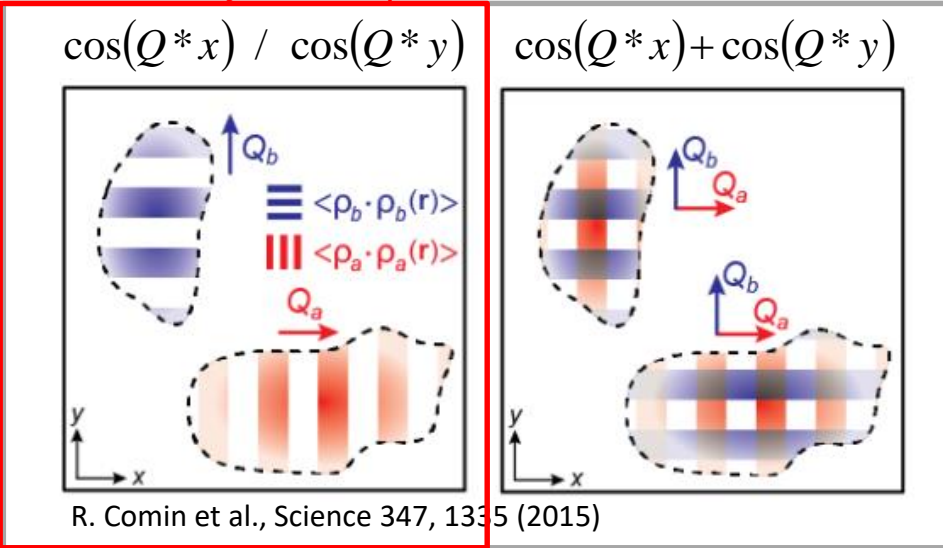
Fala gęstości ładunku (CDW) oraz fala gęstości par Coopera (PDW)

CDW – dane RXS

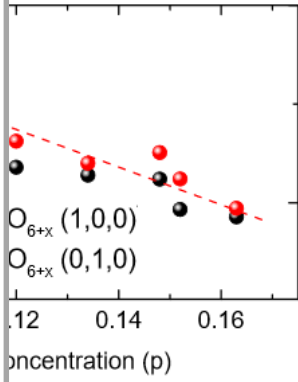


R. Comin et al., Nature

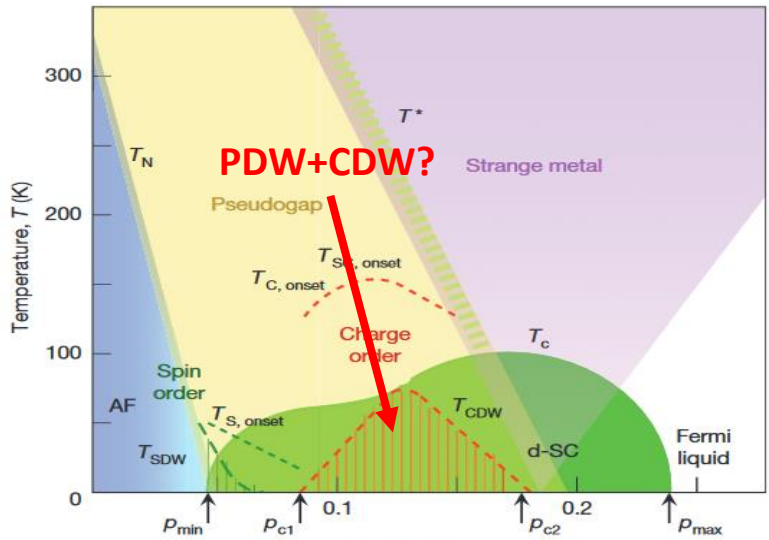
łamanie symetrii C_4



R. Comin et al., Science 347, 1335 (2015)

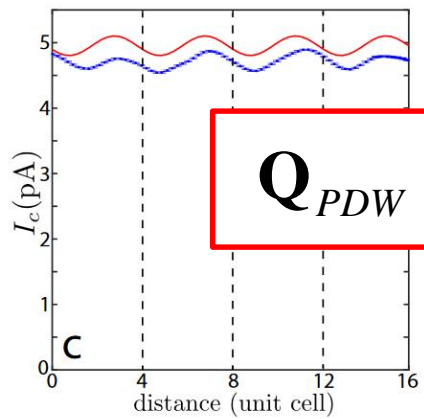


Phys. Rev. B 90, 054513 (2014)

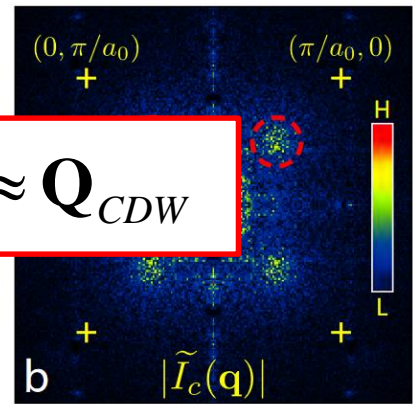


B. Keimer et al., Nature 518, 179 Hole doping, ρ

PDW – mikroskopia tunelowa Josephsona



$$Q_{PDW} \approx Q_{CDW}$$



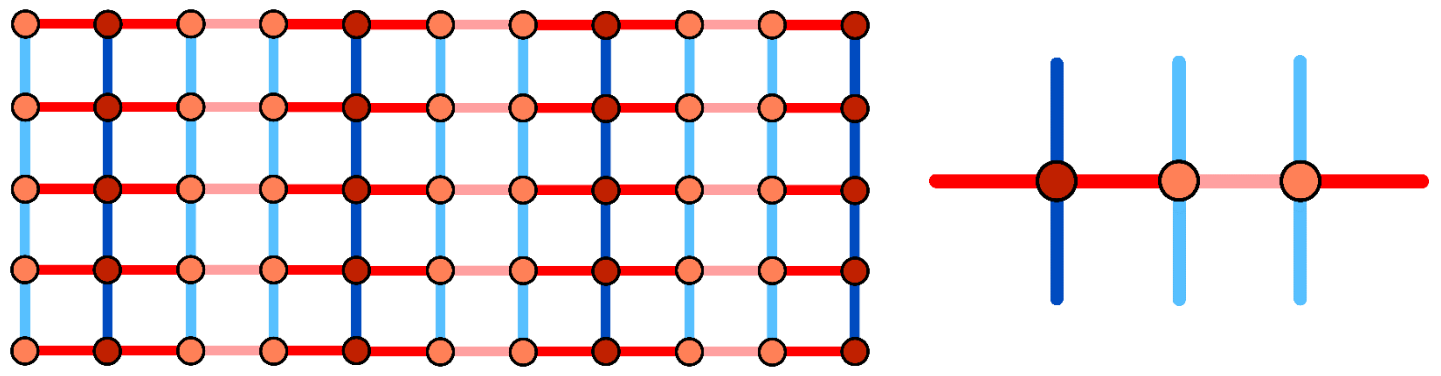
M. H. Hamidian et al., Nature 532, 343 (2016)

Fala gęstości ładunku (CDW) oraz fala gęstości par Coopera (PDW)

pairing: $\Delta_{ij} = \langle \hat{c}_{j\sigma}^+ \hat{c}_{i\sigma}^+ \rangle$

hopping: $P_{ij} = \langle \hat{c}_{j\sigma}^+ \hat{c}_{i\sigma} \rangle$

$\mathbf{Q} = (2\pi/3, 0)/a$



$$\left. \begin{aligned} \Delta_i^d &= (\Delta_{1,0} + \Delta_{-1,0} - \Delta_{0,1} + P_{0,-1})/4 \\ \Delta_i^{s'} &= (\Delta_{1,0} + \Delta_{-1,0} + \Delta_{0,1} - P_{0,-1})/4 \\ \Delta_i^x &= (\Delta_{1,0} - \Delta_{-1,0})/2 \end{aligned} \right\} \begin{aligned} \delta\Delta^{d,s'} &\neq 0 \\ \delta P^{d,s'} &\neq 0 \\ \delta n &\neq 0 \end{aligned} \Rightarrow \text{PDW + CDW}$$

Fala gęstości par Coopera:

$$\Delta_i^{d,s'} = \bar{\Delta}^{d,s'} + \delta\Delta^{d,s'} \cos \mathbf{QR}_i$$

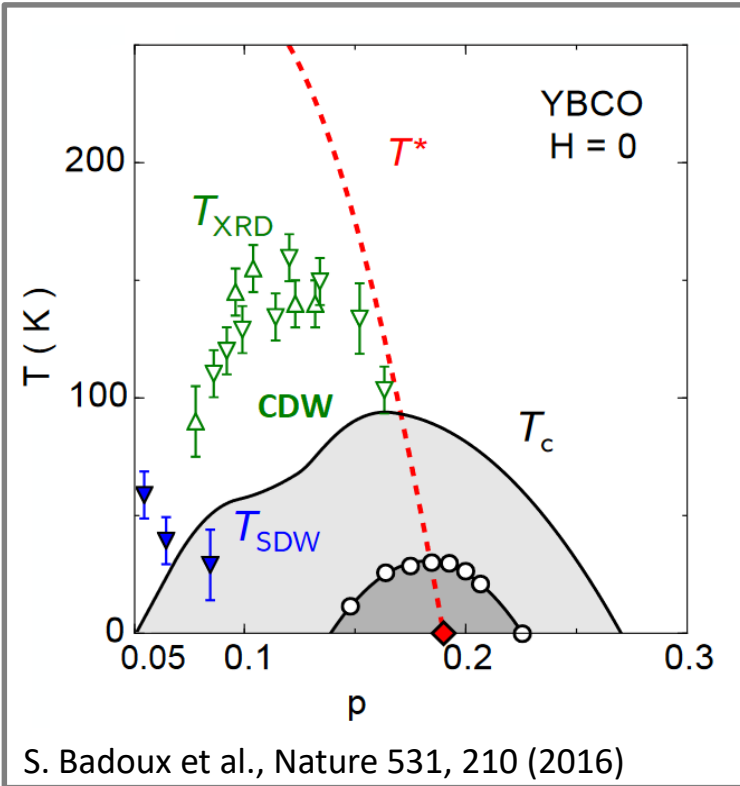
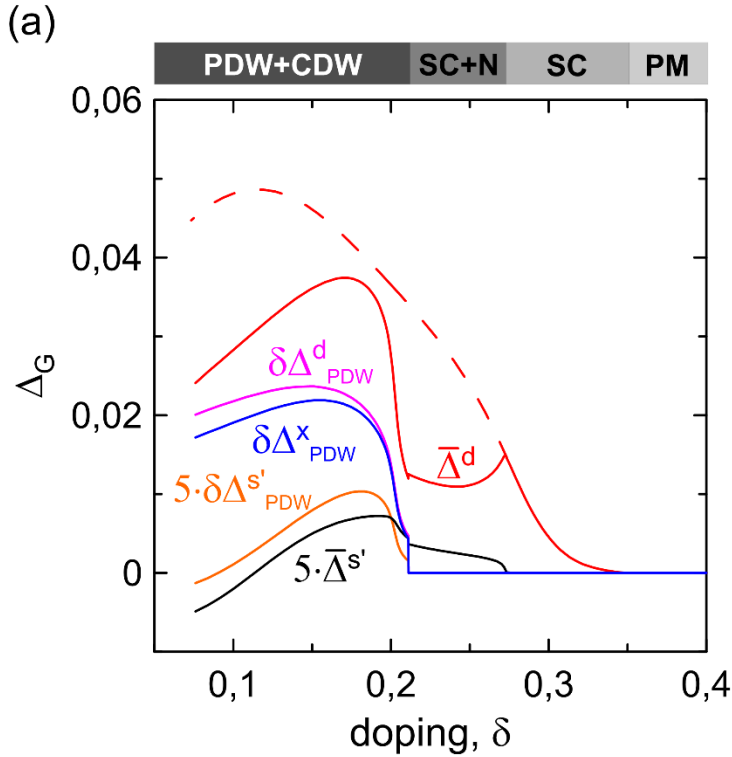
$$\Delta_i^x = \delta\Delta^x \sin \mathbf{QR}_i$$

Fala gęstości ładunku:

$$P_i^{d,s'} = \bar{P}^{d,s'} + \delta P^{d,s'} \cos \mathbf{QR}_i$$

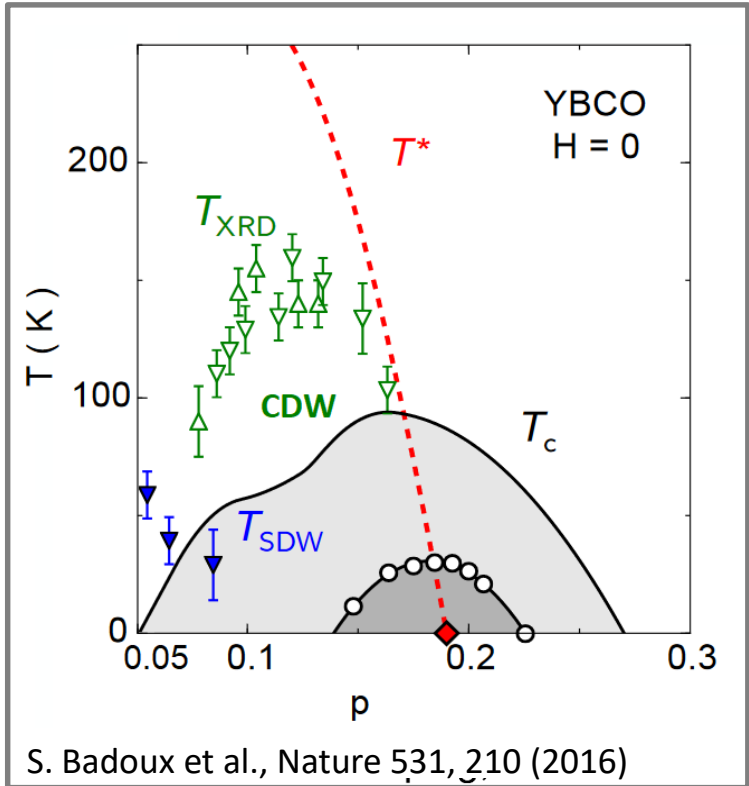
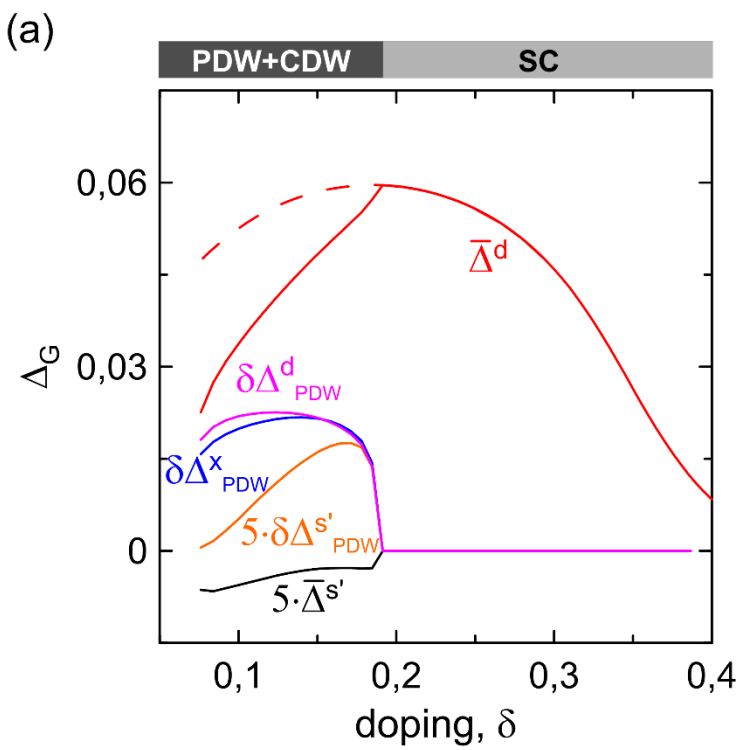
$$n_{i\sigma} = \bar{n} + \delta n \cos \mathbf{QR}_i \quad P_i^x = \delta P^x \sin \mathbf{QR}_i$$

PDW+CDW: model Hubbard



$\Delta_i^{d,s'} = \bar{\Delta}^{d,s'} + \delta \Delta^{d,s'} \cos \mathbf{QR}_i$ $\Delta_i^x = \delta \Delta^x \sin \mathbf{QR}_i$	$P_i^{d,s'} = \bar{P}^{d,s'} + \delta P^{d,s'} \cos \mathbf{QR}_i$ $P_i^x = \delta P^x \sin \mathbf{QR}_i, \quad n_{i\sigma} = \bar{n} + \delta n \cos \mathbf{QR}_i$
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PDW+CDW: model t-J-U



$$\Delta_i^{d,s'} = \bar{\Delta}^{d,s'} + \delta \Delta^{d,s'} \cos \mathbf{QR}_i$$

$$\Delta_i^x = \delta \Delta^x \sin \mathbf{QR}_i$$

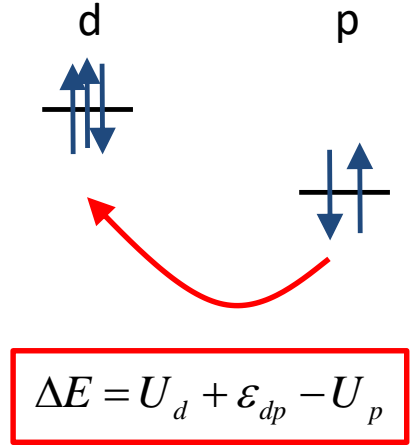
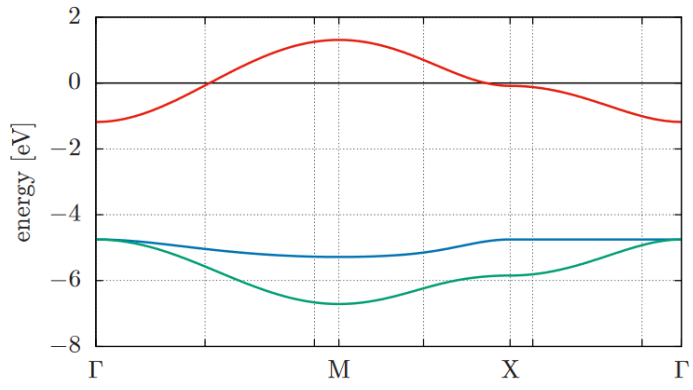
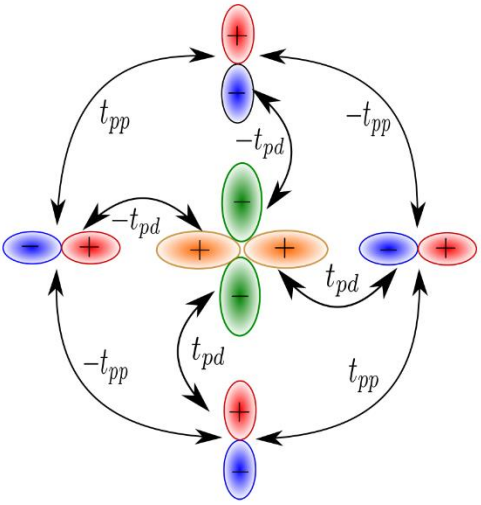
$$P_i^{d,s'} = \bar{P}^{d,s'} + \delta P^{d,s'} \cos \mathbf{QR}_i$$

$$P_i^x = \delta P^x \sin \mathbf{QR}_i, \quad n_{i\sigma} = \bar{n} + \delta n \cos \mathbf{QR}_i$$

Model trójpasmowy (d-p)

$$\hat{H} = -t_{dp} \sum_{\langle ij \rangle \sigma} (-1)_{ij} \hat{d}_{i\sigma}^+ \hat{p}_{j\sigma} - t_p \sum_{\langle ij \rangle \sigma} (-1)_{ij} \hat{p}_{i\sigma}^+ \hat{p}_{j\sigma} + \varepsilon_p \sum_i \hat{n}_{p,i} + \varepsilon_d \sum_i \hat{n}_{d,i}$$

$$+ U_d \sum_i \hat{n}_{d,i,\uparrow} \hat{n}_{d,i,\downarrow} + U_p \sum_i \hat{n}_{p,i,\uparrow} \hat{n}_{p,i,\downarrow}$$



$$t_{dp} = 1.1 - 1.5 eV$$

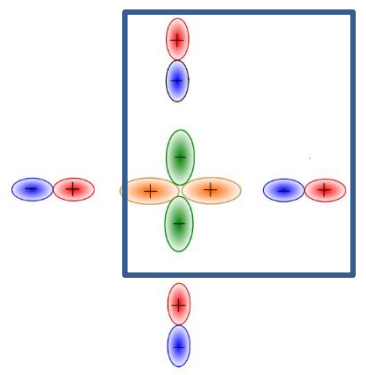
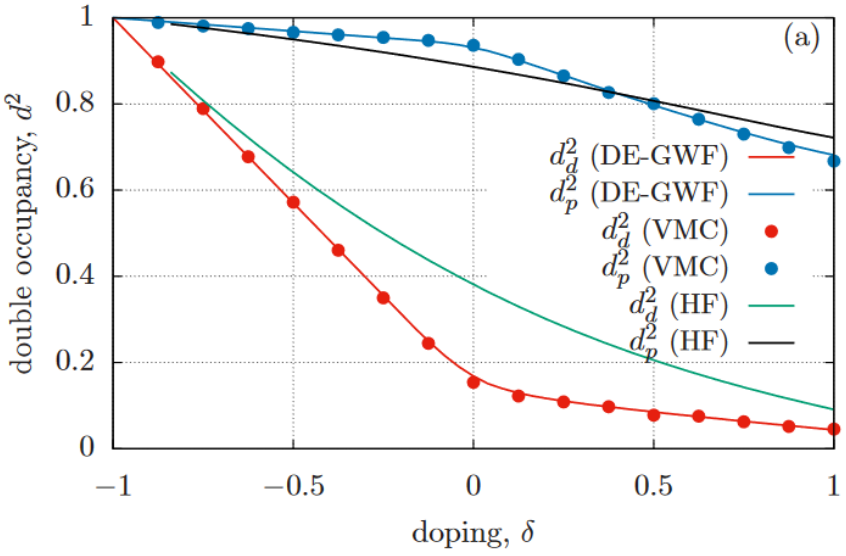
$$U_d = 8 - 10 eV$$

$$t_p = 0.5 - 0.65 eV$$

$$U_p = 4 - 5 eV$$

$$\varepsilon_{dp} = \varepsilon_d - \varepsilon_p = 1.2 - 3.5 eV$$

Model trójpasmowy (d-p): charakterystyki stanu normalnego



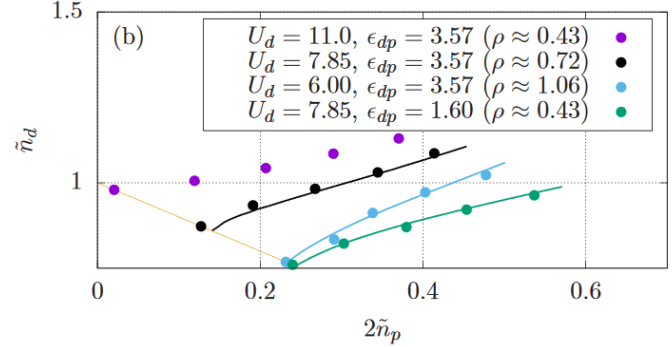
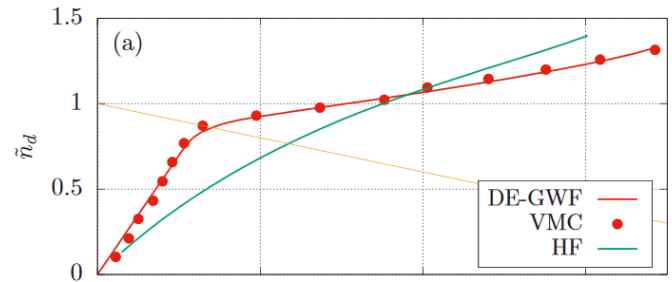
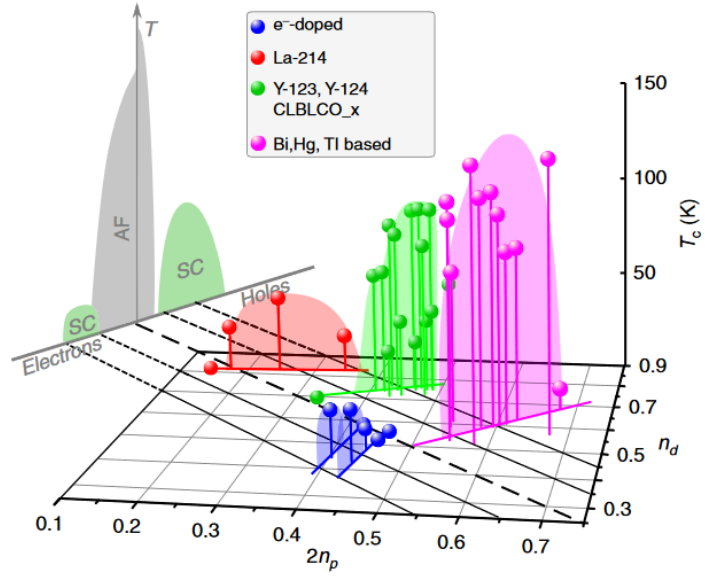
$$\delta = 5 - n_{tot}, \quad n_{tot} = n_d + 2n_p$$

$\delta > 0 \Rightarrow n_{tot} < 5$ (hole-doping)

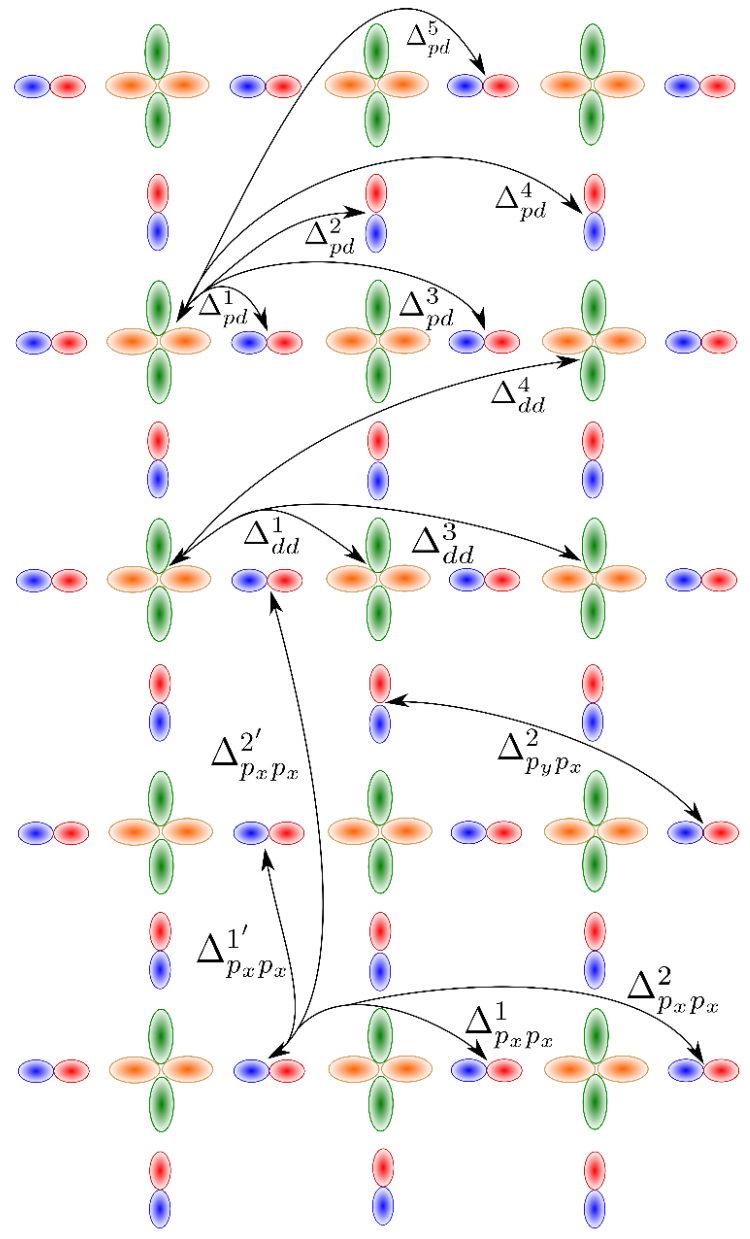
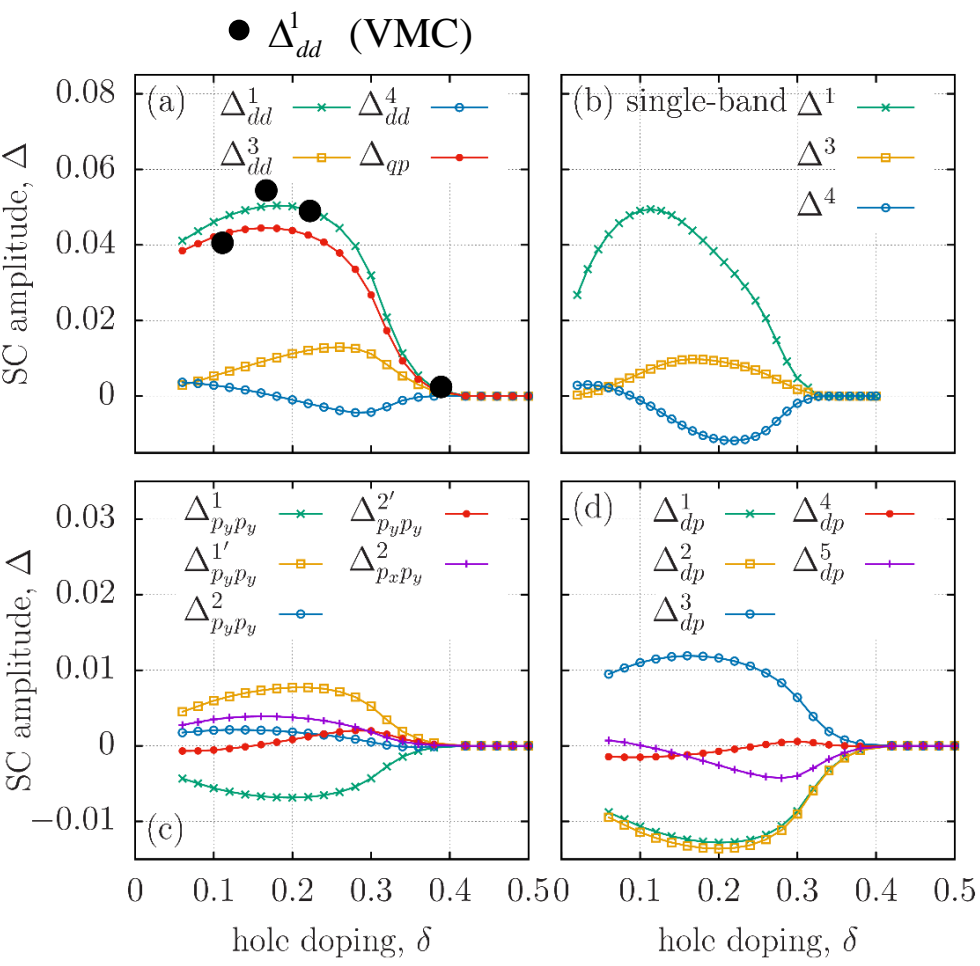
$\delta < 0 \Rightarrow n_{tot} > 5$ (electron-doping)

$$\rho = \Delta \tilde{n}_d / 2\Delta \tilde{n}_p$$

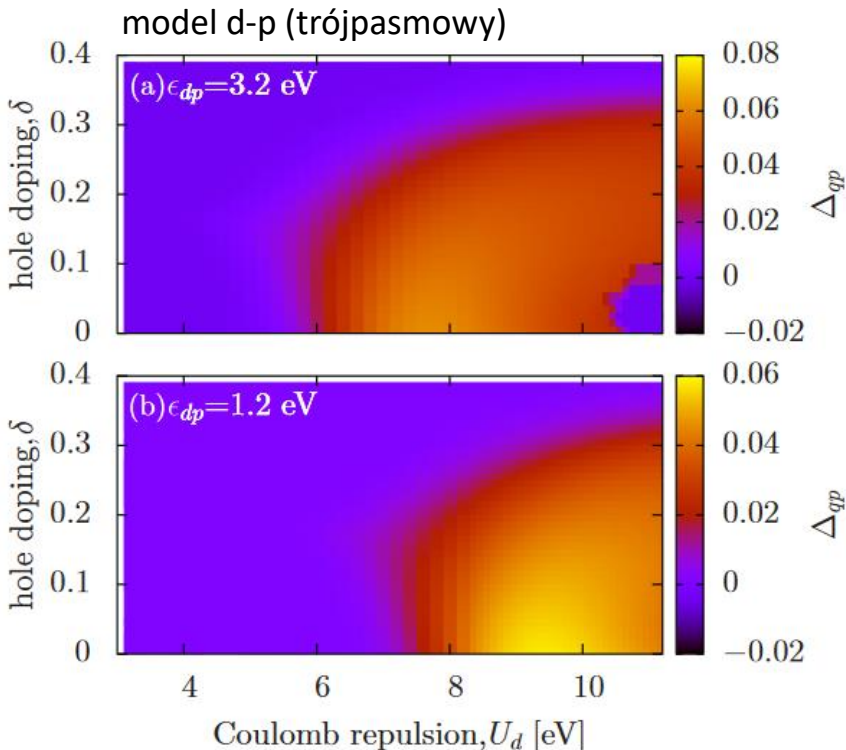
D. Rybicki et al., Nat. Commun. 7,11413(2016)



Model trójpasmowy (d-p): amplitudy parowania

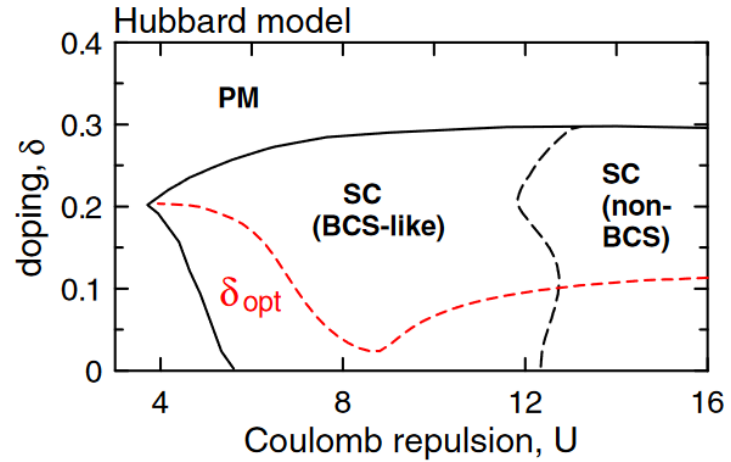
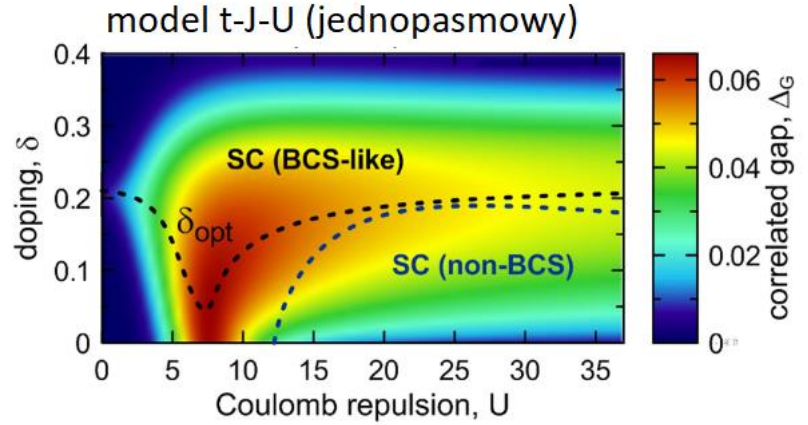


Model trójpasmowy (d-p): faza nadprzewodząca



$$\Delta E = U_d + \epsilon_{dp} - U_p$$

$$\Delta E = U$$



Podsumowanie

- Ważnymi elementami opisu SC w miedzianach są: uwzględnienie wyrazu oddziaływań kinetycznej wymiany, niezerowa lecz mała ilość podwójnych obsadzeni, uwzględnienie efektów wyższych rzędów wynikających z korelacji elektronowych → podejście oparte o model t-J-U oraz metodę DE-GWF.
- Otrzymano zgodność z dostępnymi danymi doświadczalnymi dla fundamentalnych charakterystyk stanu nadprzewodzącego w kupratkach.
- Otrzymano właściwą sekwencję faz na diagramie fazowym z nadprzewodnictwem d-wave powyżej domieszkowania optymalnego oraz modulacją ładunkową poniżej (koegzystencja PDW+CDW).
- W ogólnych aspektach podejścia jedno- oraz trój-pasmowe prowadzą do podobnych wyników dla fazy nadprzewodzącej.
- Jawne uwzględnienie tlenowych stopni swobody wydaje się konieczne w celu przeprowadzenia dokładnego opisu poszczególnych związków należących do rodziny kupratów oraz odwzorowania różnic jakie między nimi występują.

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Dziękuję za uwagę