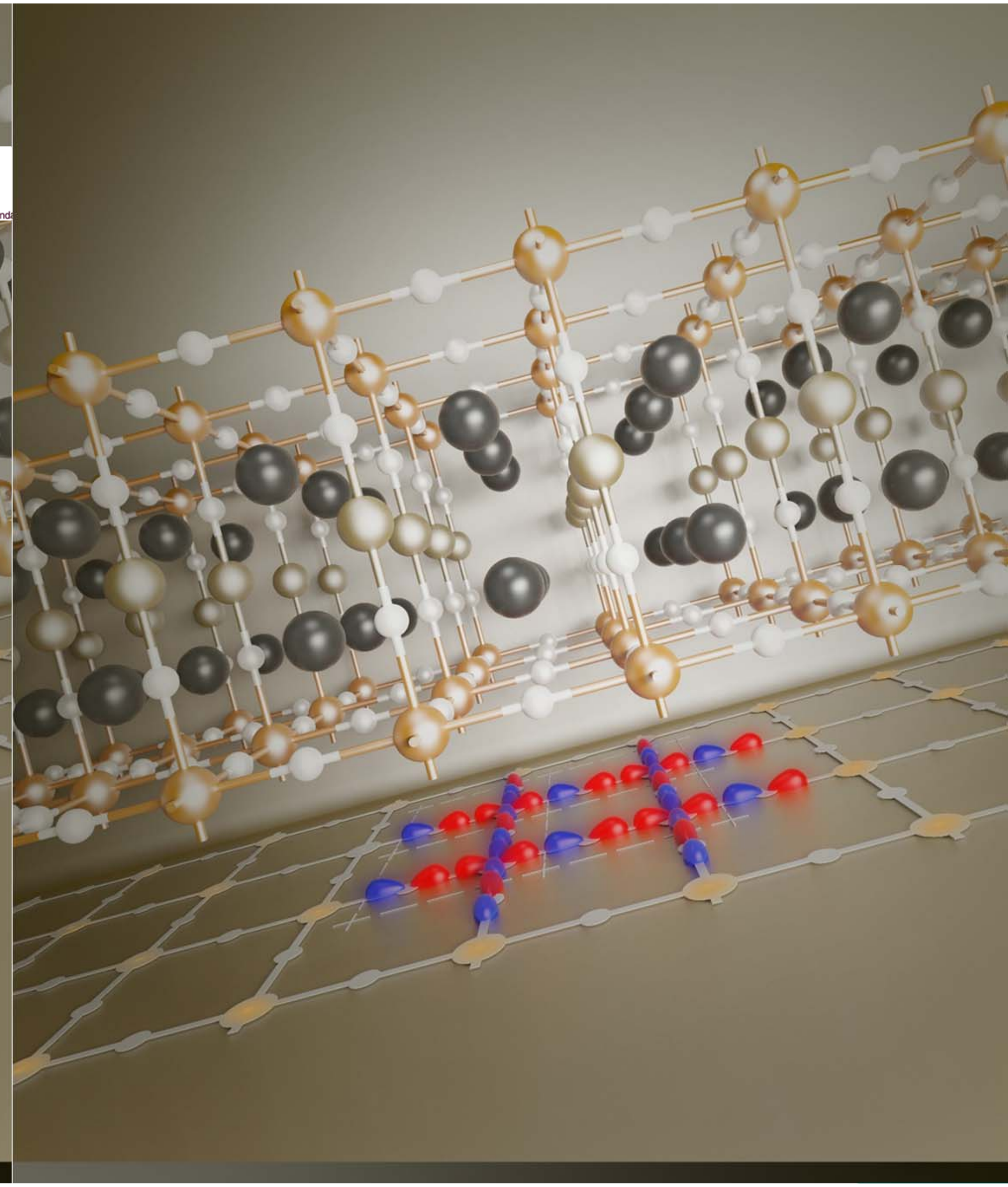
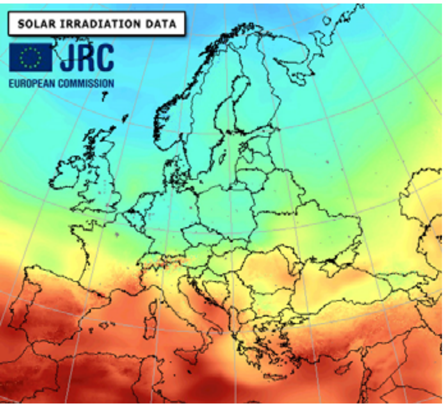
Superconducting at higher temperature : a theoretical perspective

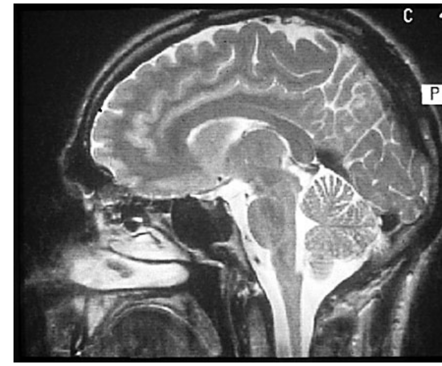
André-Marie Tremblay

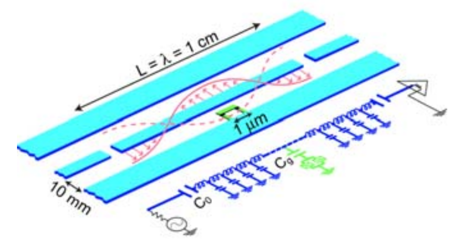
Quantum Days
8 February 2022
12:40



Applications



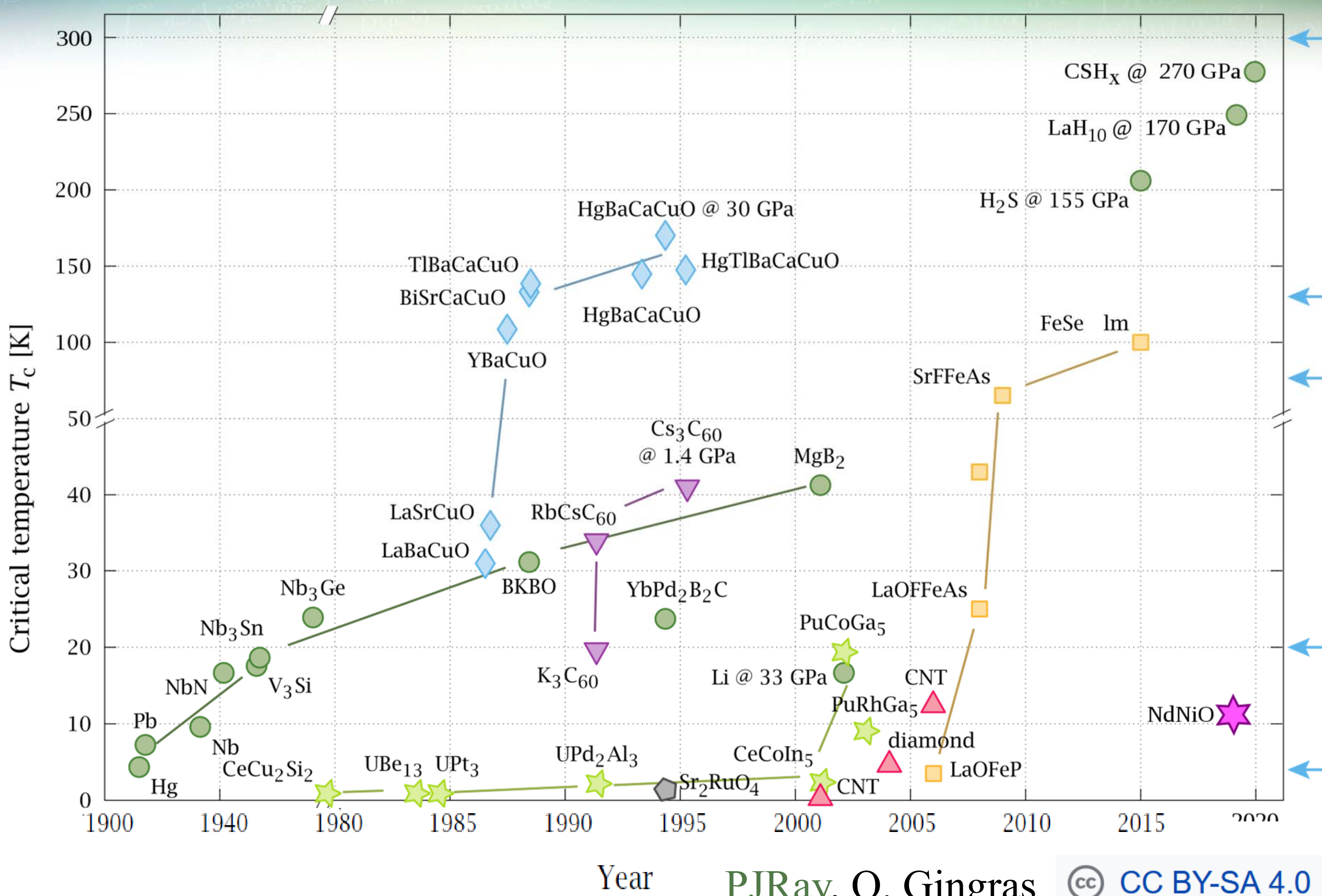




Alexandre Blais, et al. Phys. Rev. A **69**, 062320 (2004)

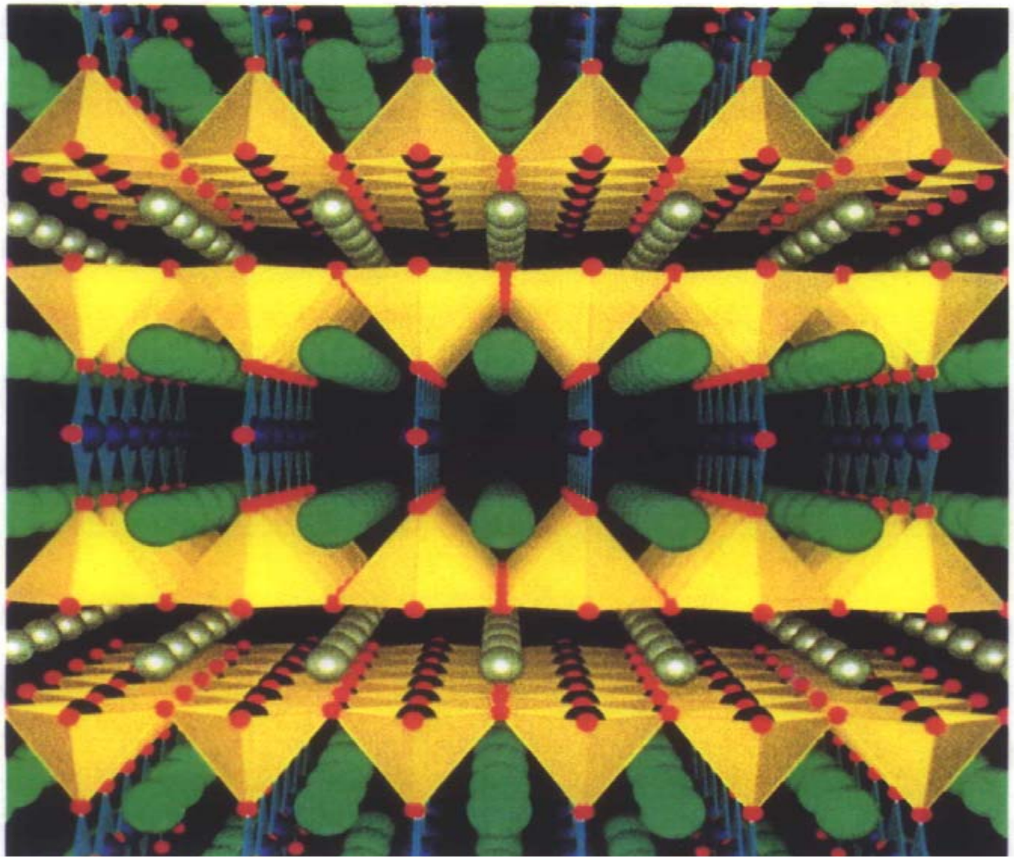
Photo IBM

Can we have superconductivity at room temperature?

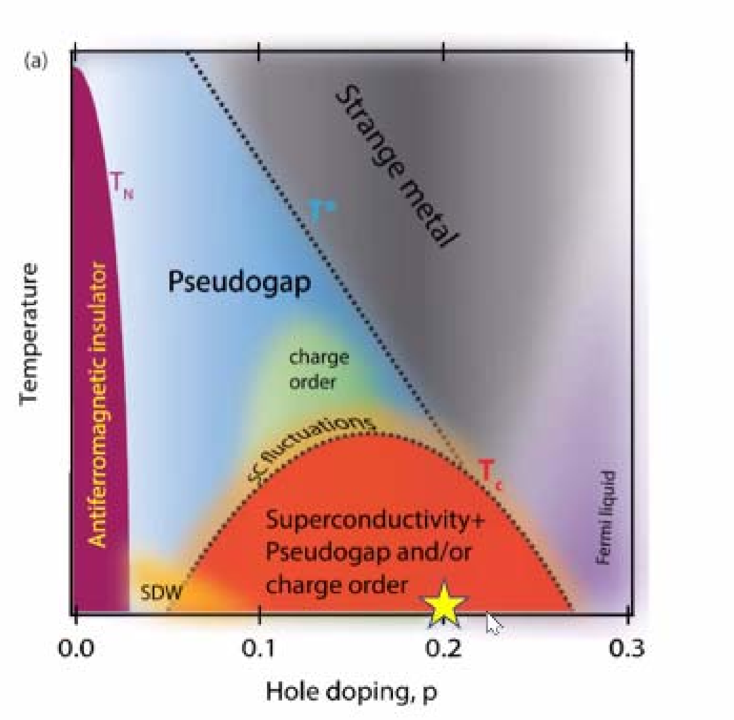


PJRay, O. Gingras

Cuprates : Atomic structure

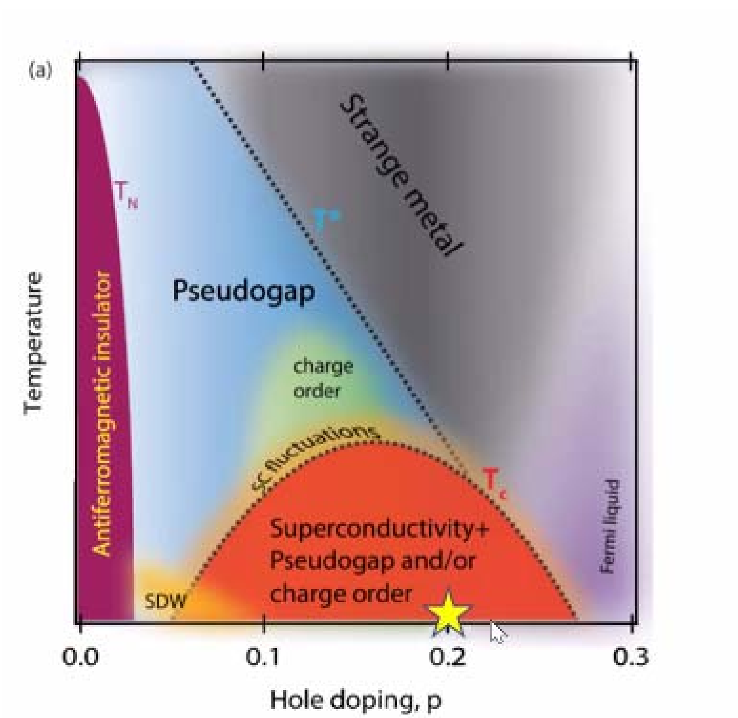


- Who ordered this?



Vishik, Rep. Prog. Phys. (2018)

- Who is looking into this?



Vishik, Rep. Prog. Phys. (2018)

A highly quantum mechanical problem

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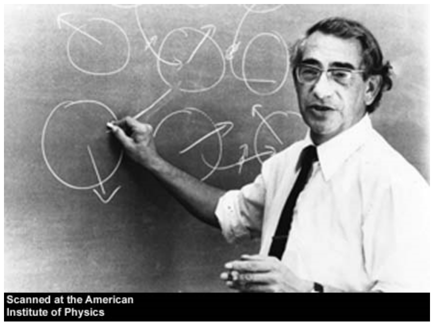
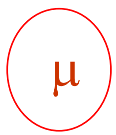
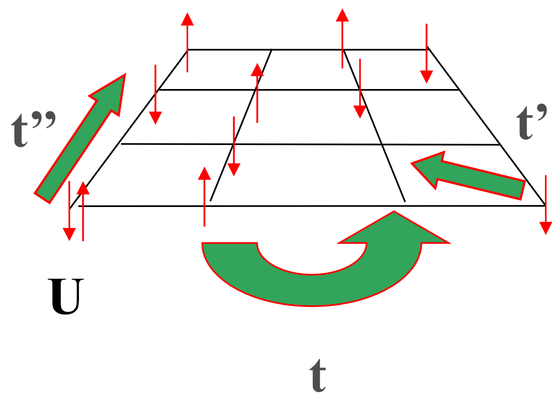
Hubbard model

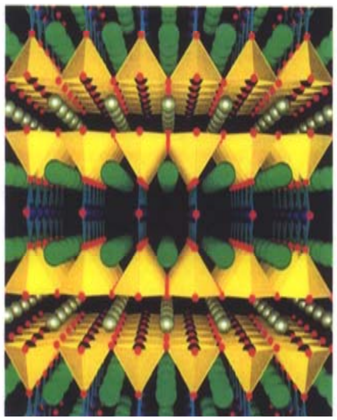


1931-1980





$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$



Spin 1/2

Attn: Charge transfer insulator

Take home messages

- A detailed picture of the origin of superconductivity in cuprates follows from a model that takes into account Cu, O, kinetic energy and interactions

- We need to look beyond traditional tools of solid state physics to work this out.

Outline

- Method
- Three-band Hubbard model
- d-wave superconductivity in cuprates

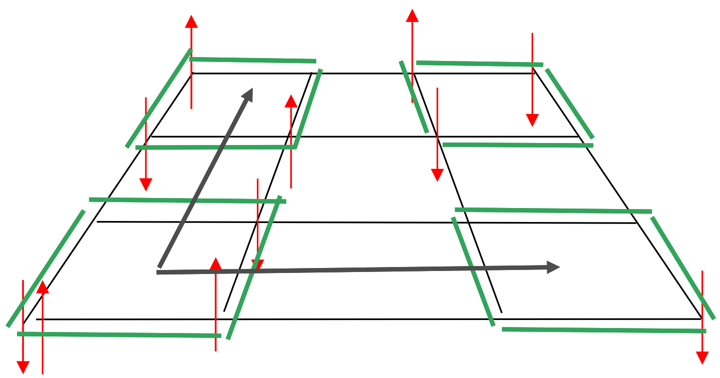
Method

Metzner, Vollhardt PRL **62**, 324 (1989)
Georges, Kotliar, PRB **45,** 6479 (1992)
Jarrell PRL **69,** 168 (1992)
Review: Georges, Kotliar, Krauth, Rozenberg, RMP **68**, 13 (1996)

Dynamical Mean-Field Theory : DMFT

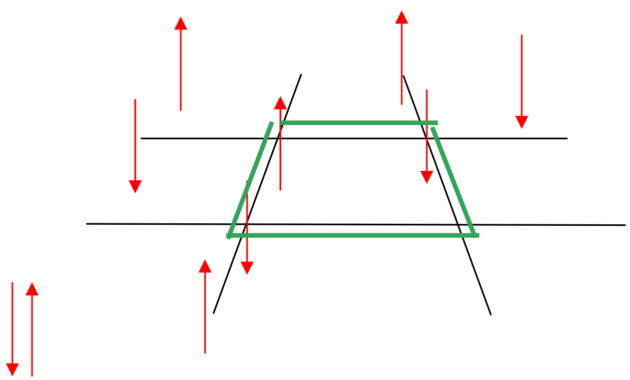
Localized and delocalized pictures C-DMFT

Delocalized



$$\mathbf{R} \rightarrow \tilde{k}$$

Localized



$$G_{ij} = \int \frac{d^d\tilde{k}}{(2\pi)^d} \left(\frac{1}{(i\omega_n+\mu)I - \varepsilon(\tilde{k}) - \Sigma} \right)_{ij}$$

$$(G^{-1})_{ij} = (G_0^{-1})_{ij} - \Sigma_{ij}$$

Three-band (Emery VSA) Hubbard model


Sidhartha Dash


Nicolas Kowalski


Patrick Sémon

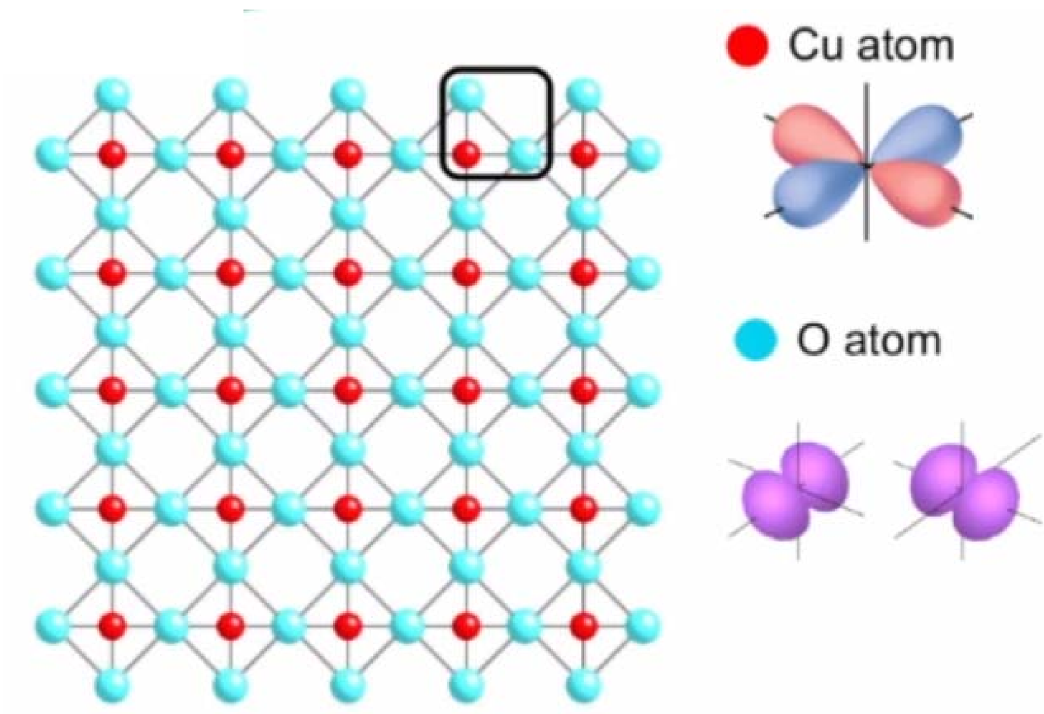

David Sénéchal

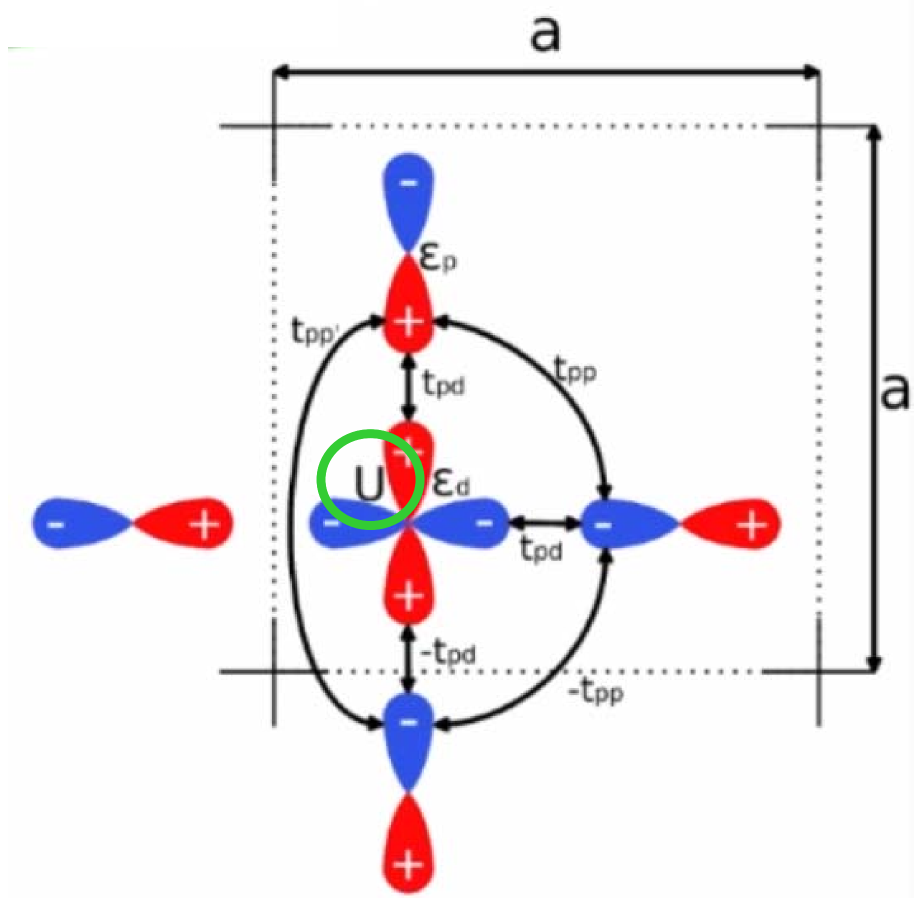
V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1987)

C. M. Varma, S. Schmitt-Rink, and E. Abrahams, Solid State Communications **62**, 681–685 (1987), ISSN 0038-1098,

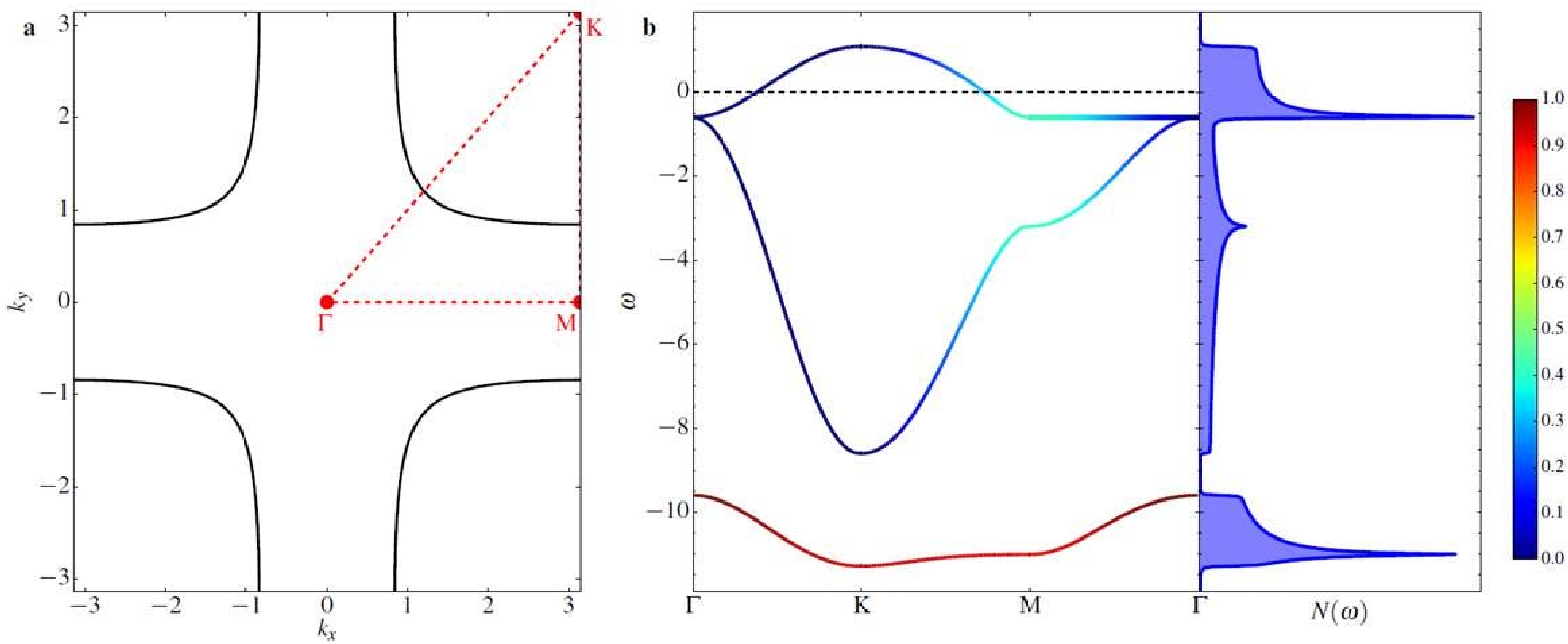
PNAS **118** (40) e2106476118 (2021)

Copper and oxygen planes



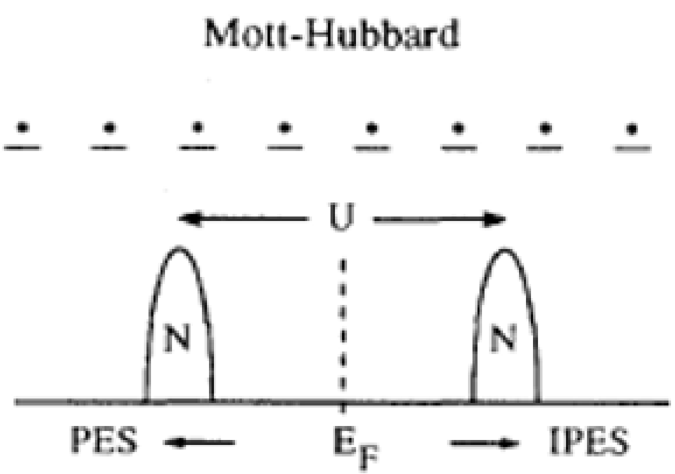


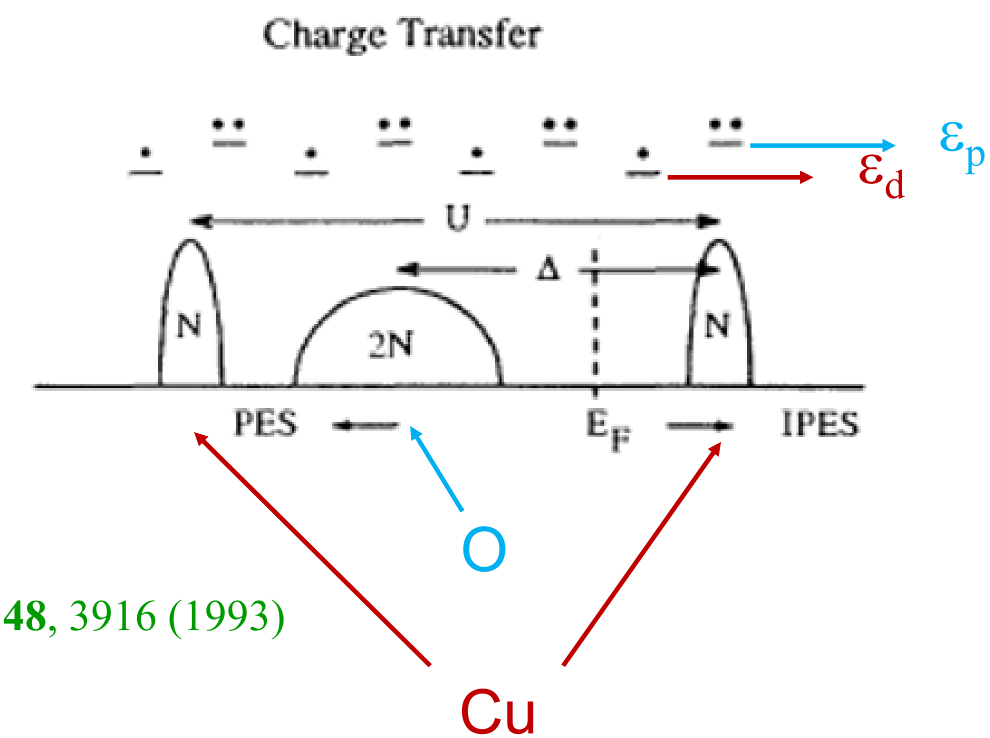
Bands : Copper-Oxygen hybridization



L. Fratino, P. Sémon, G. Sordi and A.-M.S. T.
Sci. Rep., 6, 22715 (2016)

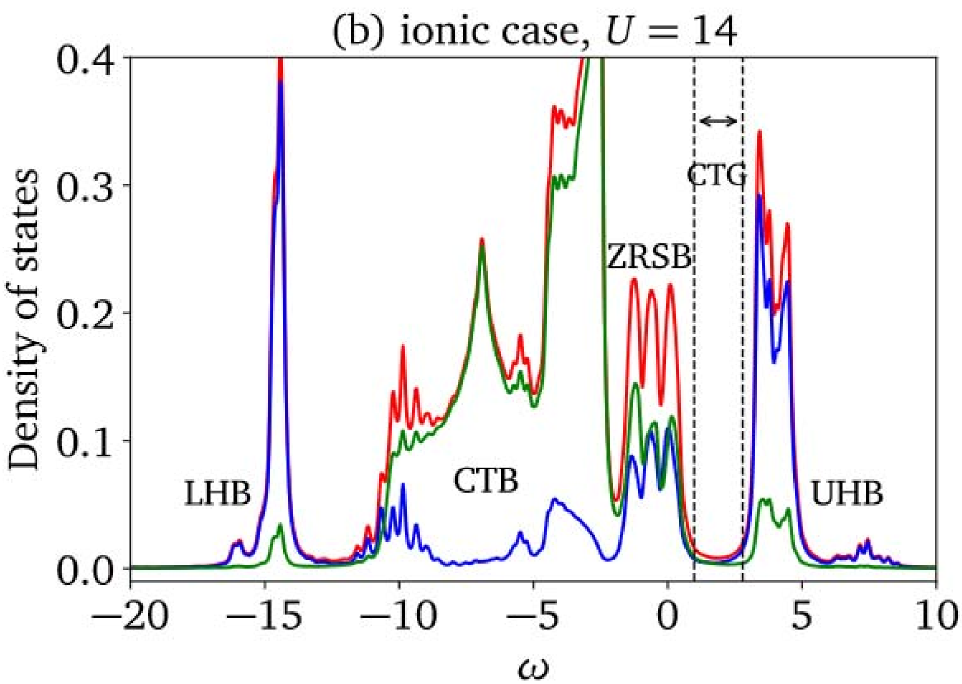
Interactions : Charge-transfer insulator

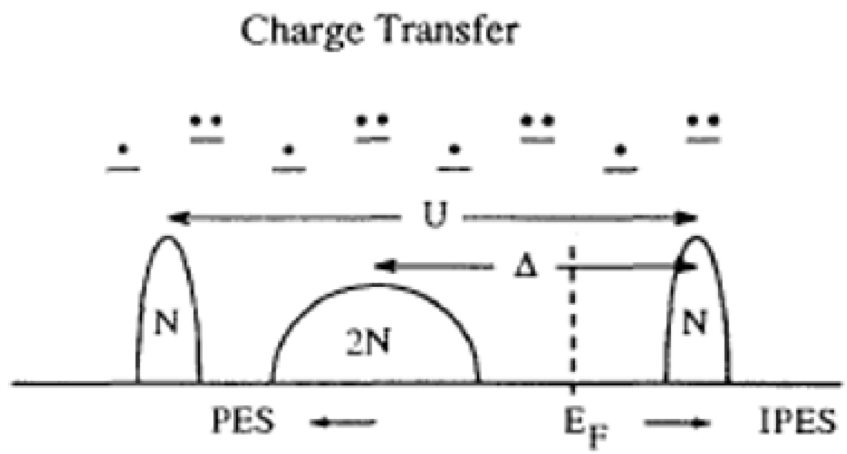




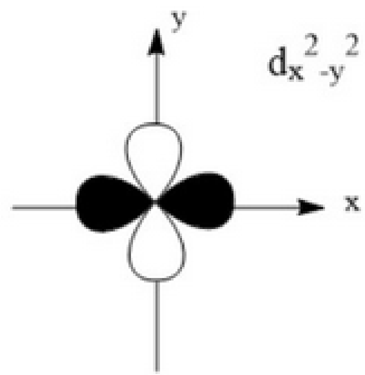
Meinders *et al*. PRB **48**, 3916 (1993)

"Ionic" limiting cases with manageable sign problem



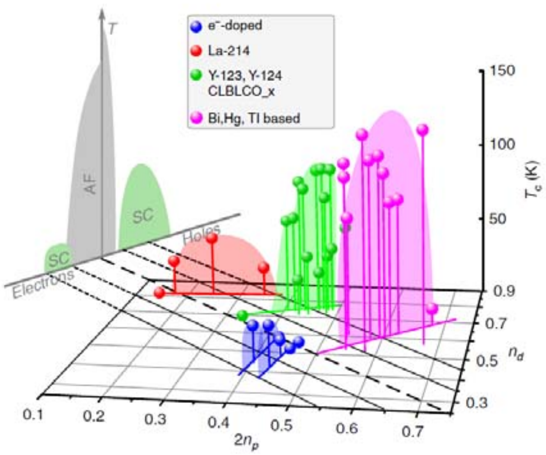


d-wave Superconductivity

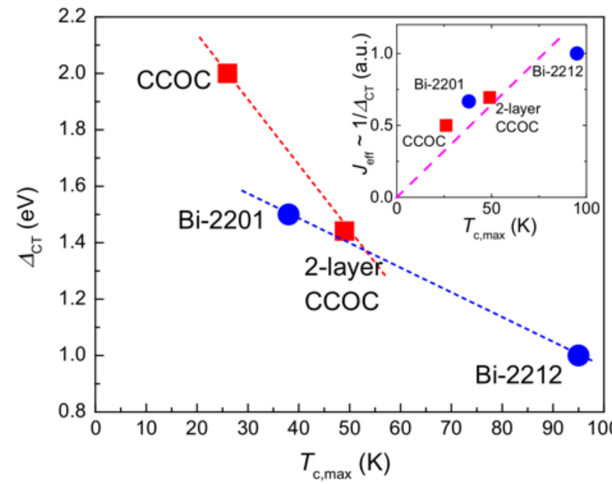


$$d = \langle \hat{d} \rangle = 1/N \sum_{\vec{k}} (\cos k_x - \cos k_y) \langle c_{\vec{k},\uparrow} c_{-\vec{k},\downarrow} \rangle$$

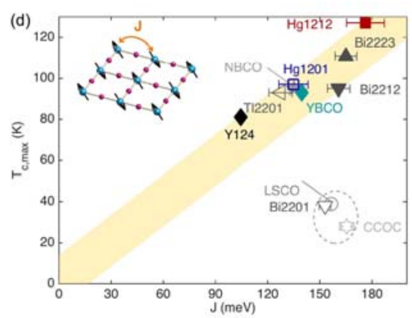
Three experimental observations



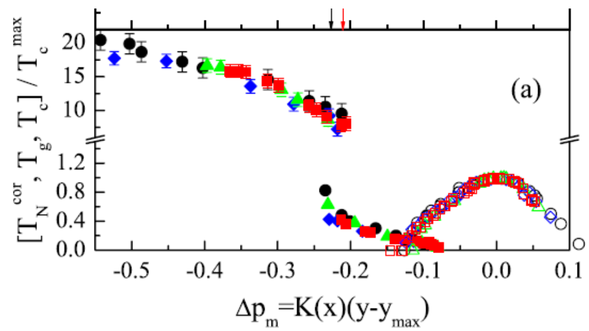
Rybicki, … Haase, Nat. Comm. 7, 11413 (2016)



Ruan *et al.* Sci. Bull. **61** (2016)

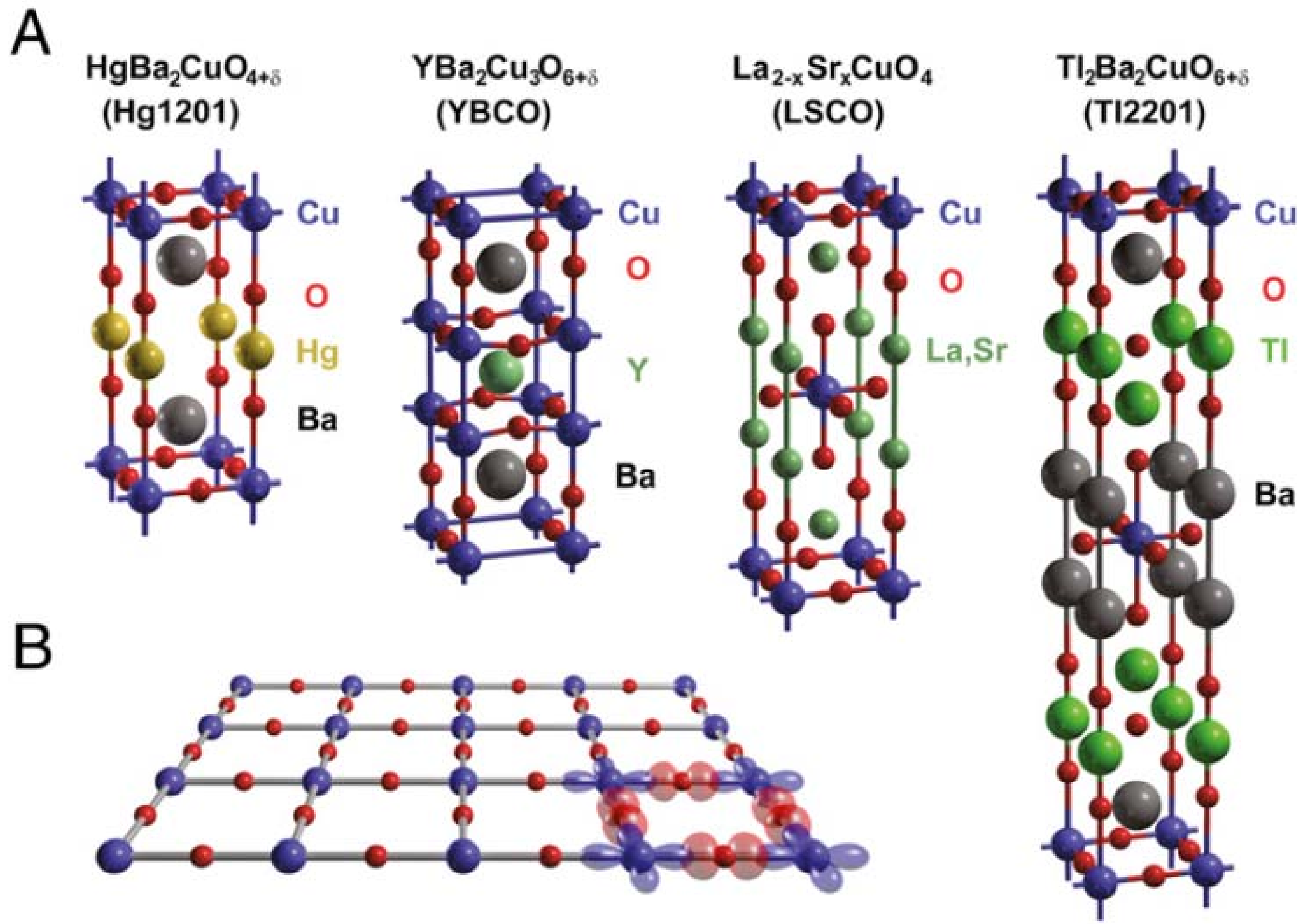


Lichen Wang, *et al.* arXiv 2011.05029

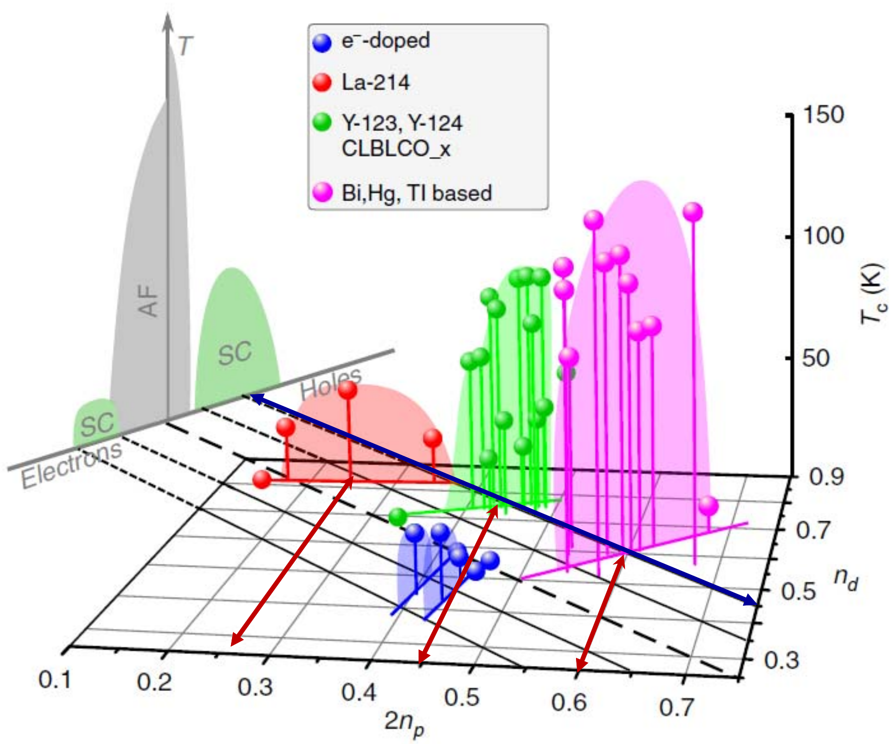


A. Keren New J. Phys. **11** 065006

There are different kinds of cuprates : All with CuO_2 planes



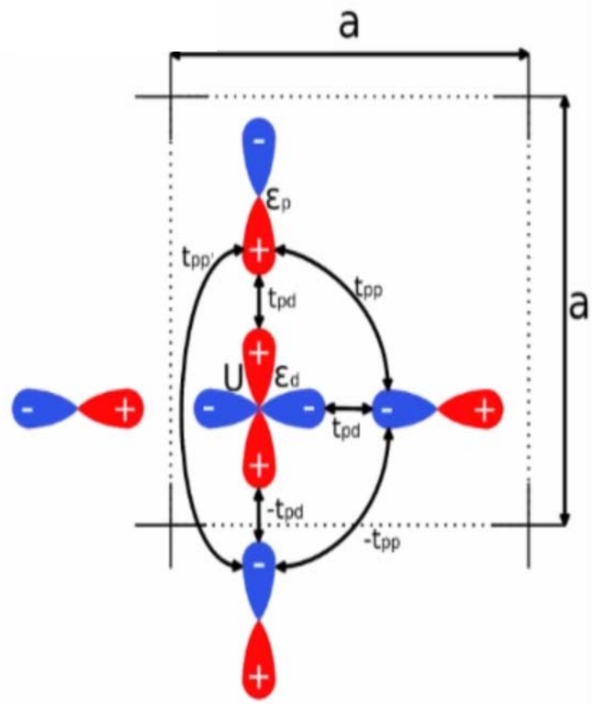
#1 Optimizing T_c with oxygen hole content



Rybicki,,, Haase, Nat. Comm. 7, 11413 (2016)

Electronic structure

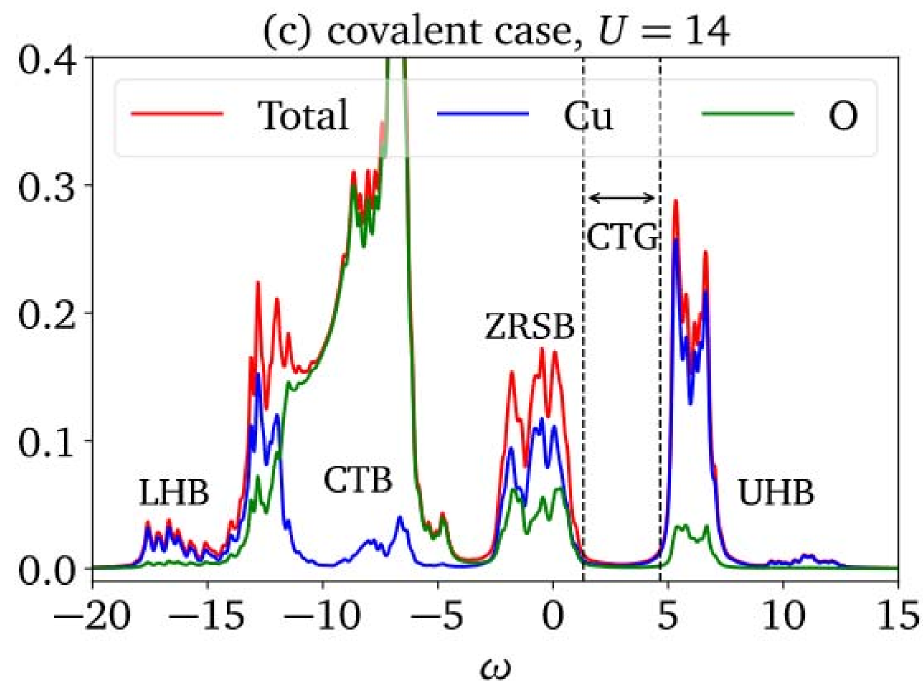
	Compound	$\epsilon_d - \epsilon_p$ (eV)	t_{pd} (eV)	t_{pp} (eV)	$t_{pp'}$ (eV)	t'/t	layers	$d^{\mathrm{apical}}_{\mathrm{Cu-O}}$ (Å)	T_c (K)
(1)	La_2CuO_4	2.61	1.39	0.640	0.103	0.070	1	2.3932	38
(2)	$Pb_2Sr_2YCu_3O_8$	2.32	1.30	0.673	0.160	0.108	2	2.3104	70
(3)	$Ca_2CuO_2Cl_2$	2.21	1.27	0.623	0.132	0.085	1	2.7539	26
(4)	$La_2CaCu_2O_6$	2.20	1.31	0.644	0.152	0.120	2	2.2402	45
(5)	$Sr_2Nd_2NbCu_2O_{10}$	2.10	1.25	0.612	0.144	0.110	2	2.0450	28
(6)	$Bi_2Sr_2CuO_6$	2.06	1.36	0.677	0.153	0.105	1	2.5885	24
(7)	$YBa_2Cu_3O_7$	2.05	1.28	0.673	0.150	0.110	2	2.0936	93
(8)	$HgBa_2CaCu_2O_6$	1.93	1.28	0.663	0.187	0.133	2	2.8053	127
(9)	$HgBa_2CuO_4$	1.93	1.25	0.649	0.161	0.122	1	2.7891	90
(10)	$Sr_2CuO_2Cl_2$	1.87	1.15	0.590	0.140	0.108	1	2.8585	30
(11a)	$HgBa_2Ca_2Cu_3O_8$ (outer)	1.87	1.29	0.674	0.184	0.141	3	2.7477	135
(11b)	$HgBa_2Ca_2Cu_3O_8$ (inner)	1.94	1.29	0.656	0.167	0.124	3	2.7477	135
(12)	$Tl_2Ba_2CuO_6$	1.79	1.27	0.630	0.150	0.121	1	2.7143	90
(13)	$LaBa_2Cu_3O_7$	1.77	1.13	0.620	0.188	0.144	2	2.2278	79
(14)	$Bi_2Sr_2CaCu_2O_8$	1.64	1.34	0.647	0.133	0.106	2	2.0033	95
(15)	$Tl_2Ba_2CaCu_2O_8$	1.27	1.29	0.638	0.140	0.131	2	2.0601	110
(16a)	$Bi_2Sr_2Ca_2Cu_3O_{10}$ (outer)	1.24	1.32	0.617	0.159	0.138	3	1.7721	108
(16a)	$Bi_2Sr_2Ca_2Cu_3O_{10}$ (inner)	2.24	1.32	0.678	0.198	0.121	3	1.7721	108



© Nicolas Kowalski

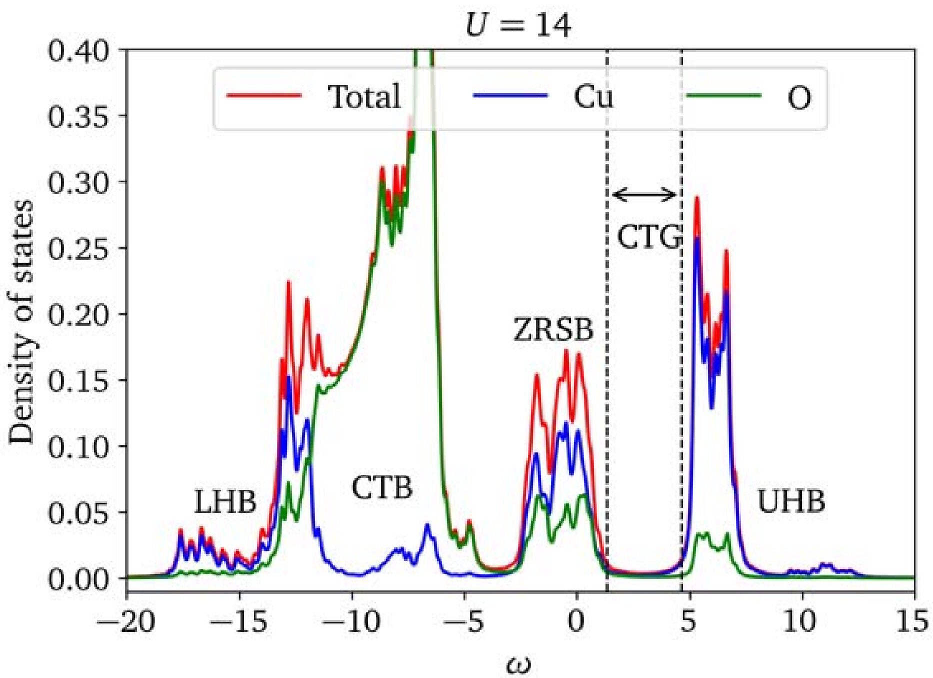
Weber, Yee, Haule, Kotliar, EPL 100, 2012

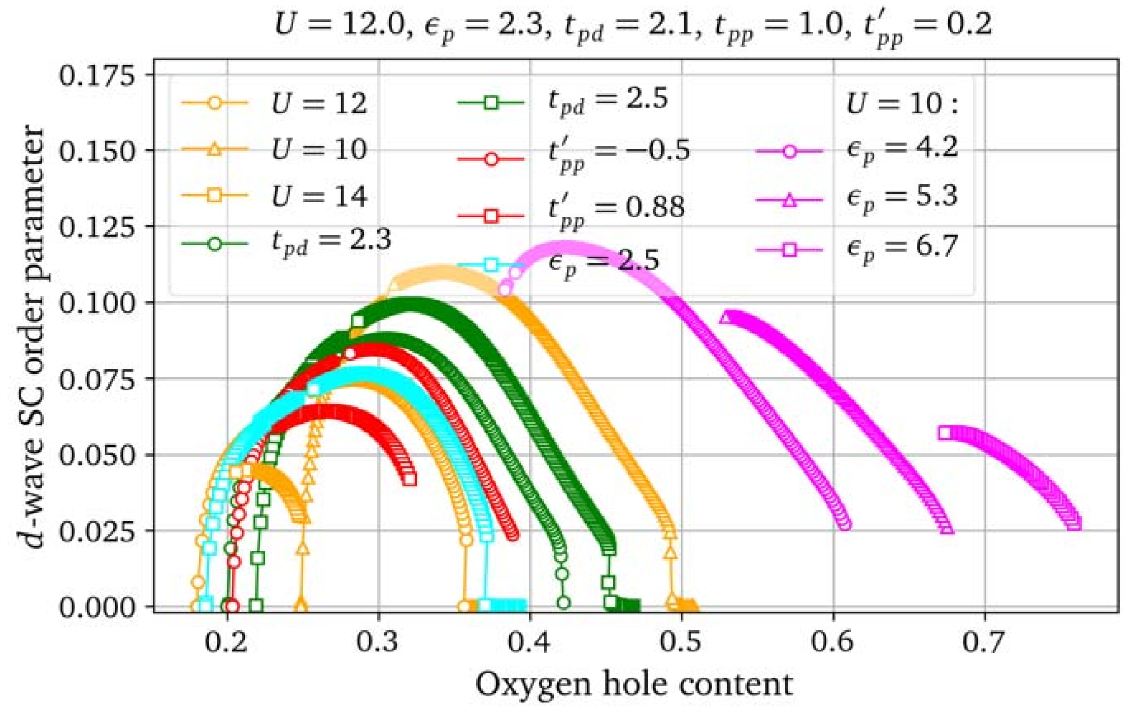
Density of states



○ $\varepsilon_p - \varepsilon_d = 2.3$, $t_{pd} = 2.1$, $t_{pp} = 1.0$, $t'_{pp} = 0.2$

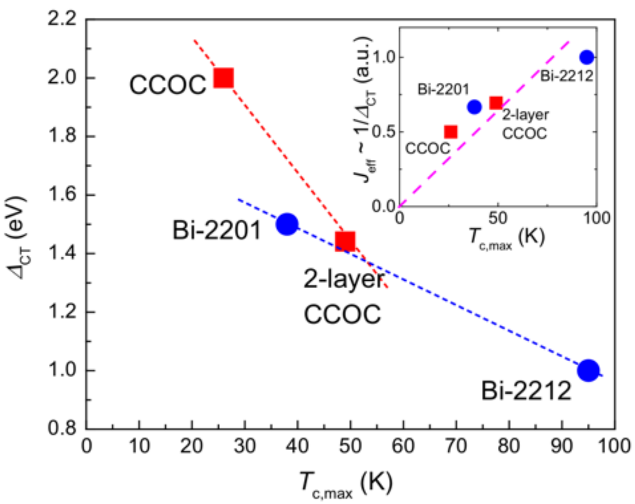
T = 0 superconducting domes for the covalent model



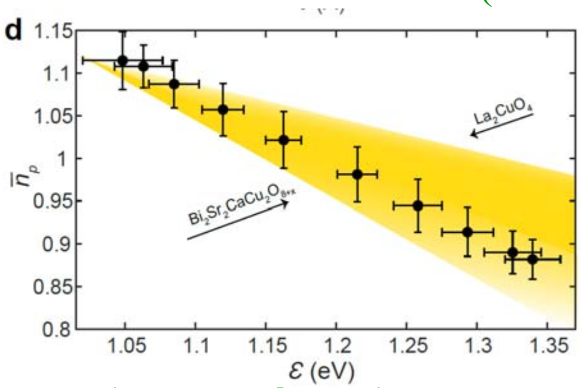


Kowalski, Dash, Sémon, Sénéchal, A-M.T.
PNAS **118** (40) e2106476118 (2021)

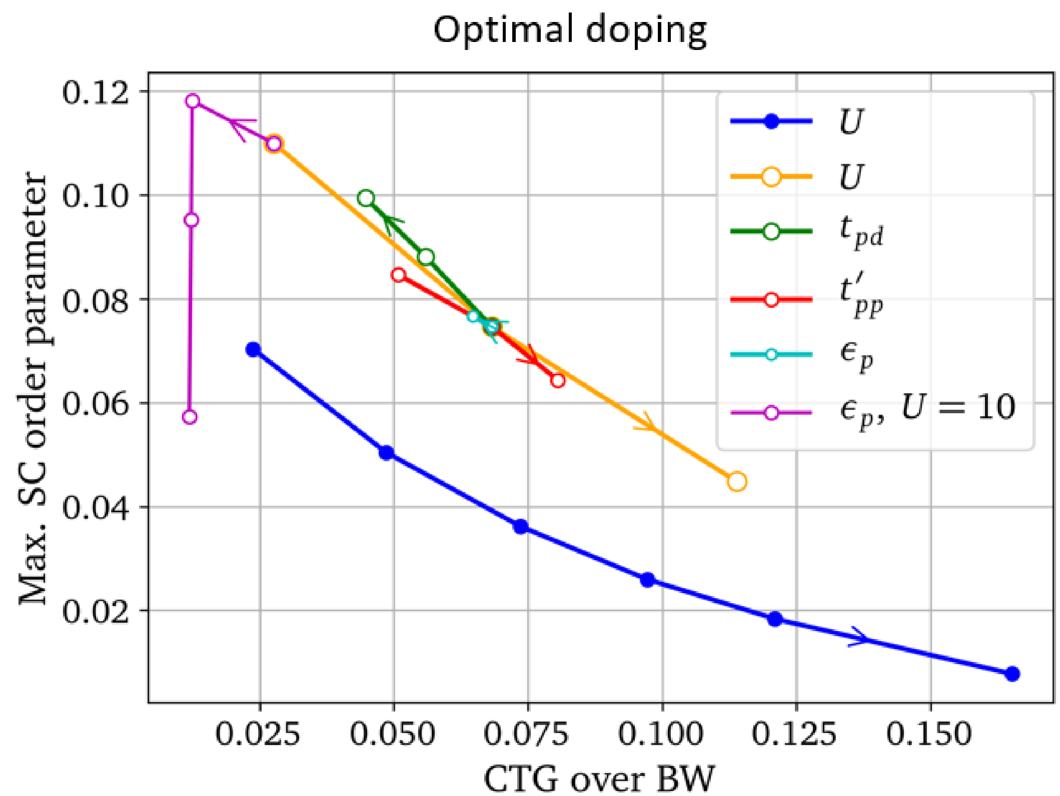
#2 Optimizing T_c with CT gap Δ (Oxygen as a witness)



Ruan *et al.* Sci. Bull. **61** (2016)

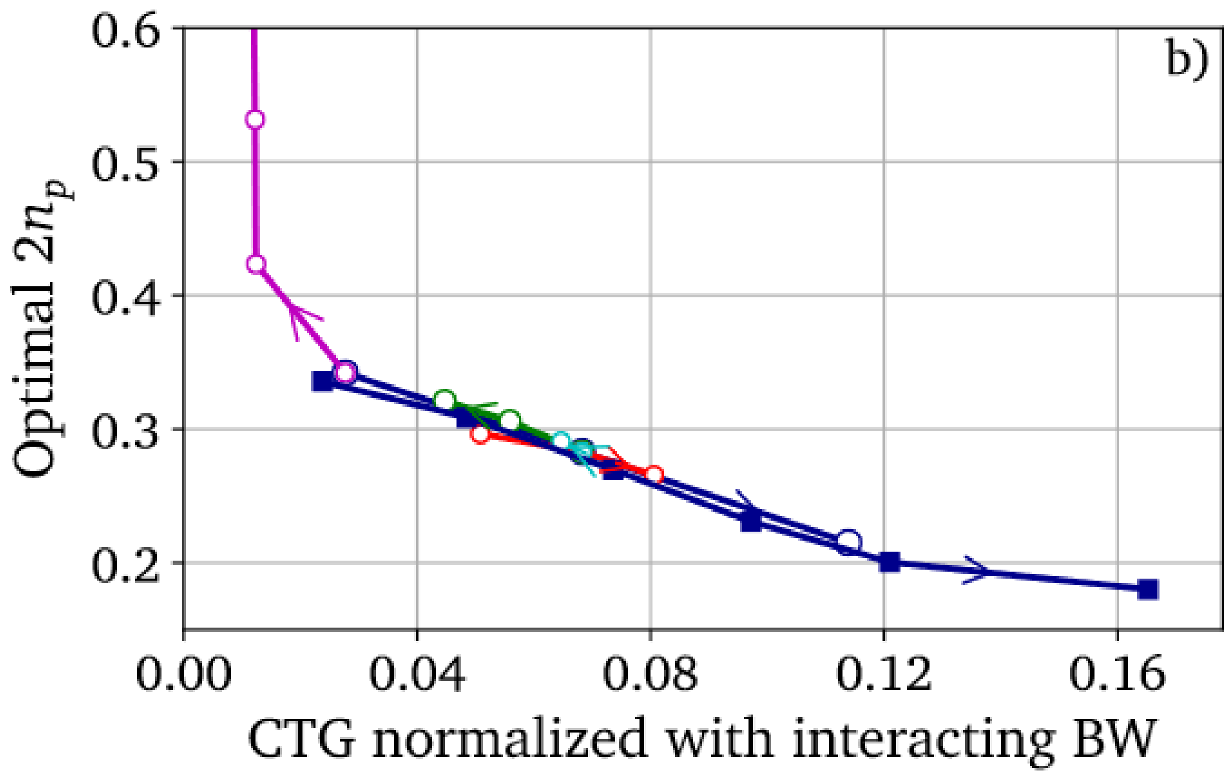


O'Mahony *et al.* arXiv:2108.03655



Kowalski, Dash, Sémon, Sénéchal, A-M.T.
PNAS **118** (40) e2106476118 (2021)

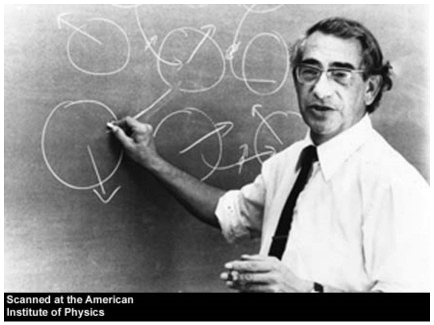
Charge-transfer gap, oxygen hole content

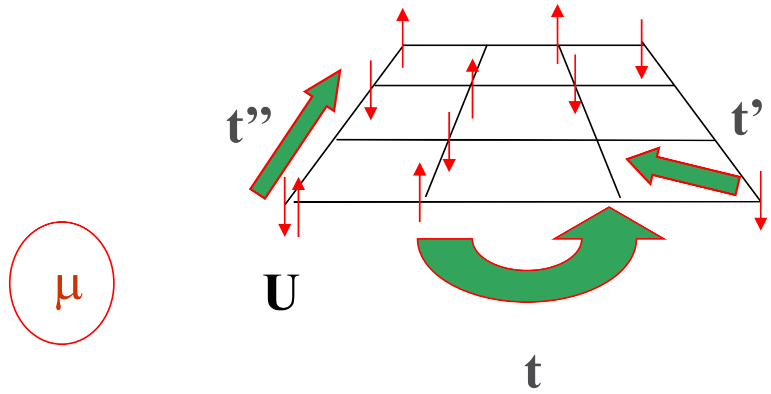


Kowalski, Dash, Sémon, Sénéchal, A-M.T.
PNAS **118** (40) e2106476118 (2021)

Copper pairing mechanism : superexchange

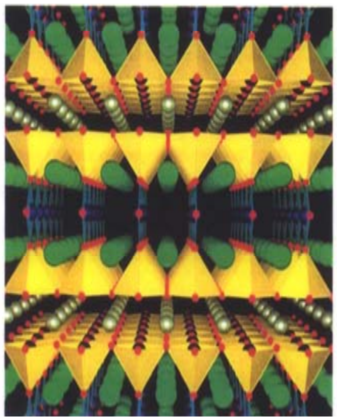
Hubbard model



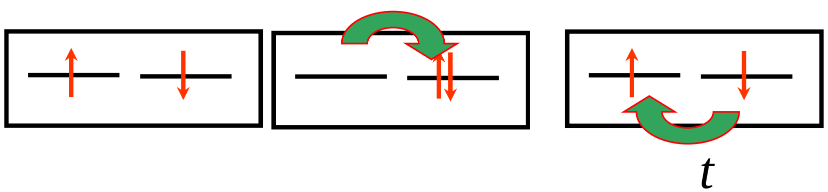


1931-1980

$$H = -\sum_{<ij>\sigma} t_{i,j}\left(c^{\dagger}_{i\sigma}c_{j\sigma} + c^{\dagger}_{j\sigma}c_{i\sigma}\right) + U\sum_{i} n_{i\uparrow}n_{i\downarrow}$$



Spin 1/2



Effective model, Heisenberg: $J = 4t^2/U$

Attn: Charge transfer insulator

A cartoon strong correlation picture

$$J \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{S}_j = J \sum_{\langle i,j \rangle} \left(\frac{1}{2} c_i^\dagger \vec{\sigma} c_i \right) \cdot \left(\frac{1}{2} c_j^\dagger \vec{\sigma} c_j \right)$$

$$d = \langle \hat{d} \rangle = 1/N \sum_{\vec{k}} (\cos k_x - \cos k_y) \langle c_{\vec{k},\uparrow} c_{-\vec{k},\downarrow} \rangle$$

$$H_{MF} = \sum_{\vec{k},\sigma} \varepsilon(\vec{k}) c^\dagger_{\vec{k},\sigma} c_{\vec{k},\sigma} - 4Jm\hat{m} - Jd(\hat{d} + \hat{d}^\dagger) + F_0$$

Pitaevskii Brückner:

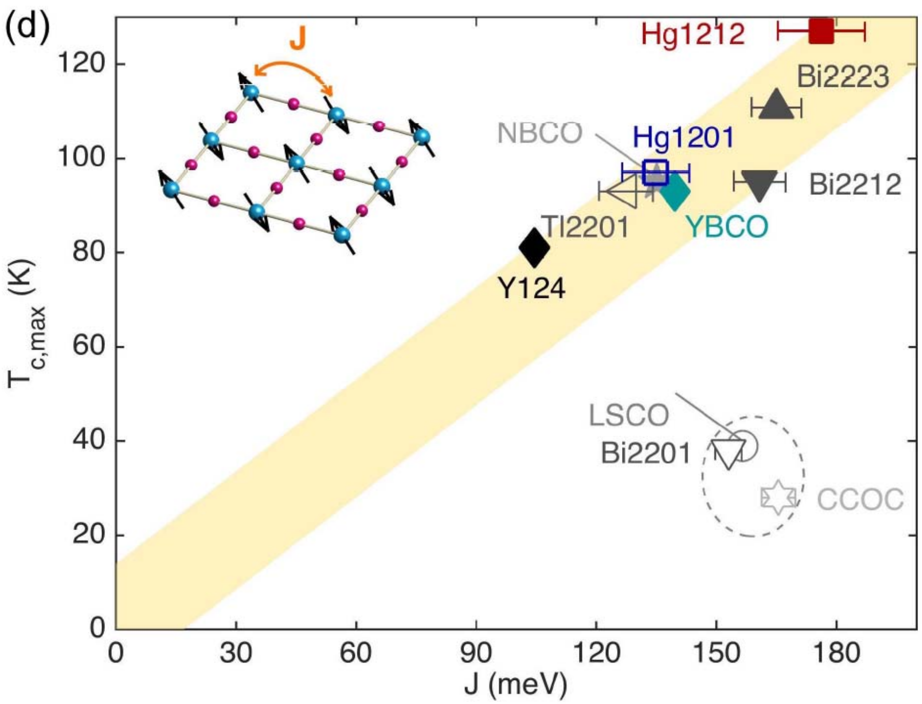
Pair state orthogonal to repulsive core of Coulomb interaction

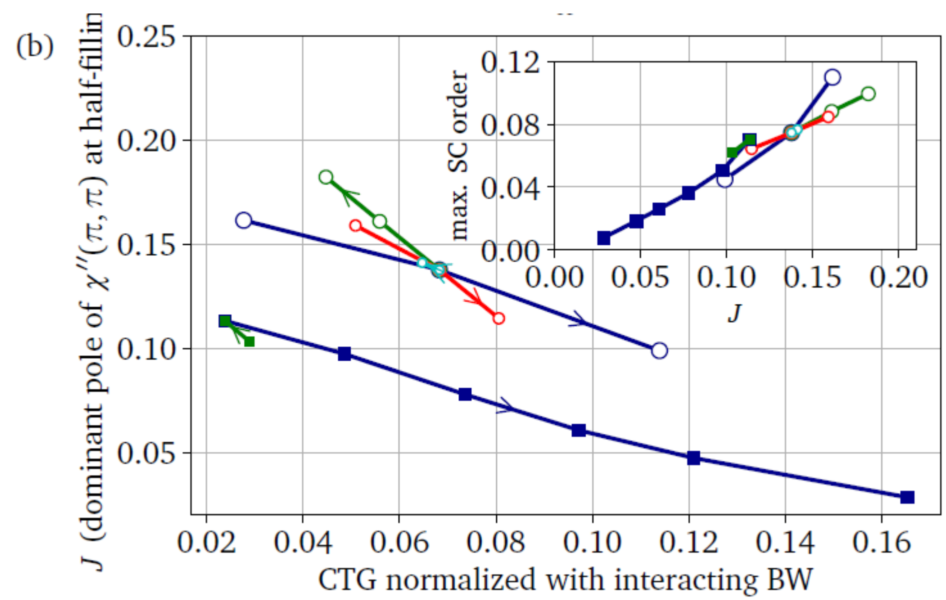
P.W. Anderson Science 317, 1705 (2007)

Miyake, Schmitt–Rink, and Varma P.R. B **34**, 6554-6556 (1986)

More sophisticated Slave Boson: Kotliar Liu PRB 1988

#3 Optimizing T_c with superexchange



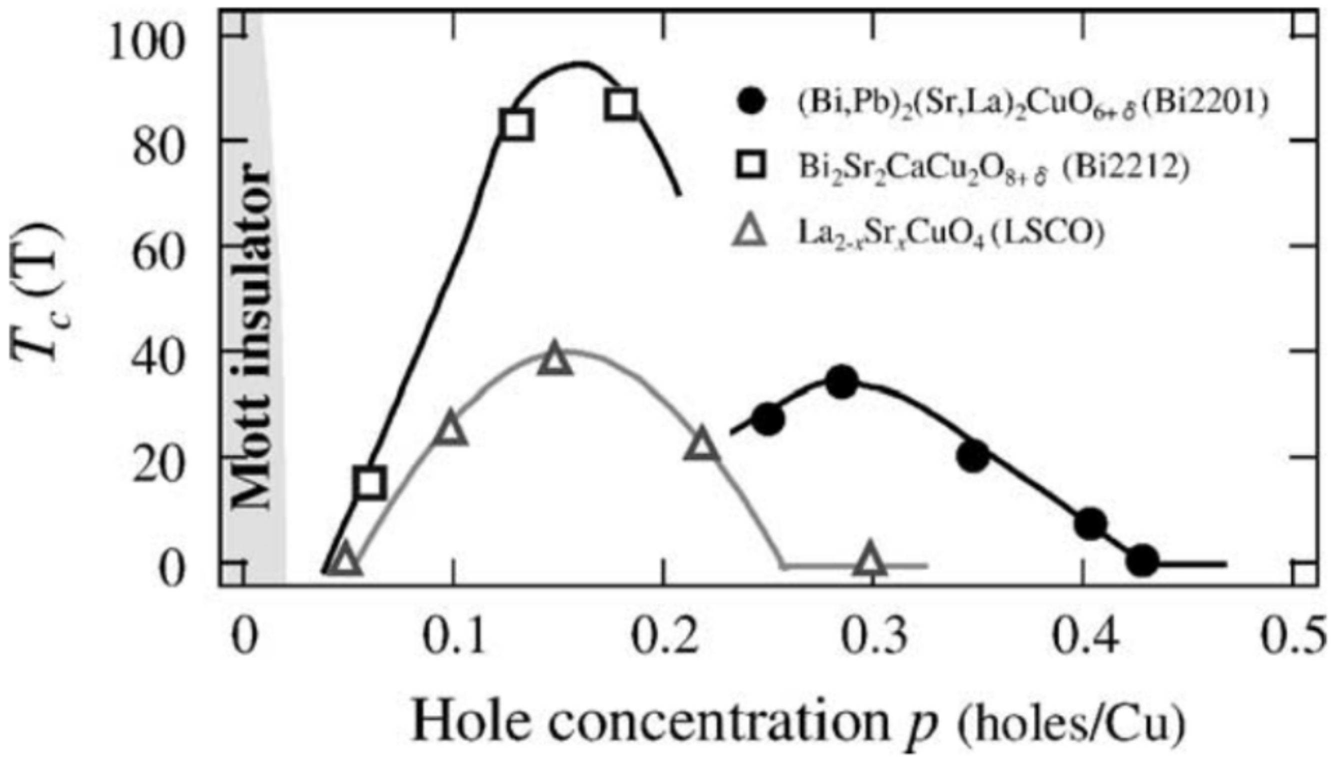


Lichen Wang, *et al.* arXiv 2011.05029

$J = 4t^2 / U$

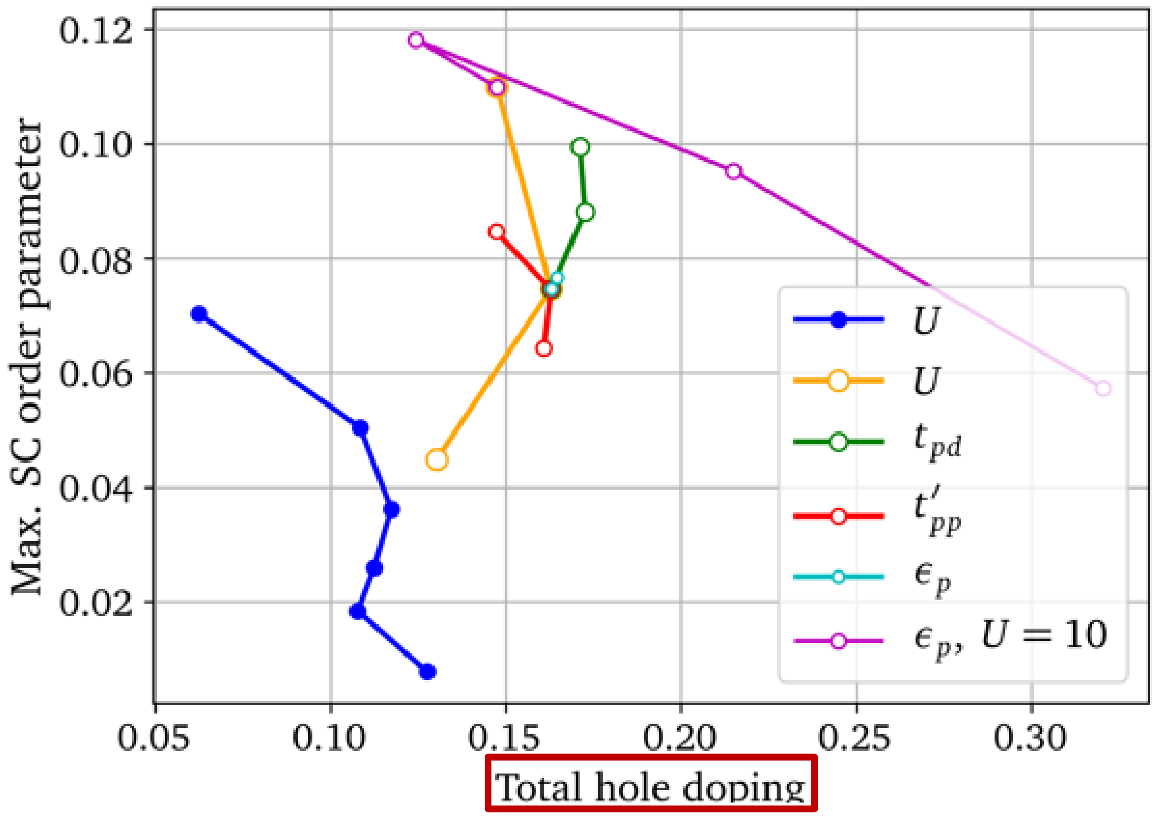
Bonus

T_c and total hole concentration are not well correlated



T. Kondo *et al.*
Journal of Electron Spectroscopy and Related Phenomena **137-140**, 663 (2004)

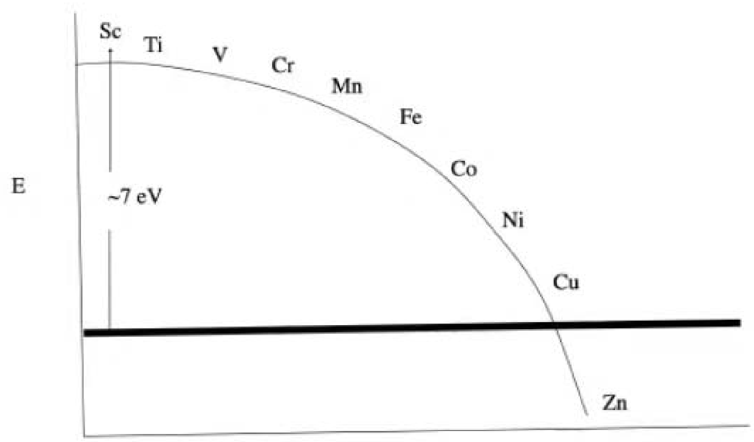
Bonus: total hole doping does not explain max order parameter for the two models



Kowalski, Dash, Sémon, Sénéchal, A-M.T.
PNAS **118** (40) e2106476118 (2021)

Bonus : Importance of covalency

Affinity Energy ($E(M^{2+}) - E(M^{1+})$) of first row Trans. Metals in relation to Ionization Energy of Oxygen ($E(O^{2-}) - E(O^{1-})$)



Also, Zaanen, Sawatzky, Allen (prl 1985).

C. M. Varma and T. Giamarchi, *Model for copper oxide metals and superconductors* (Elsevier Science B.V., 1995).

Summary Conclusion

Optimizing Tc

- Spin ½
- One band
- Two-dimensions
- Strong covalency between chalchogen and transition metal.
  - Chalcogen screens U
- Charge-transfer gap just opening (intermediate interactions).
- Large J at half-filling
- … and more

Chuck-Hou Yee *et al EPL* **111** 17002 (2015)

Stanev *et al.*, npj Computational Materials **4**, 29 (2018)

Liu *et al*. APL Materials **8**, 061104 (2020)

Merci
Thank you

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