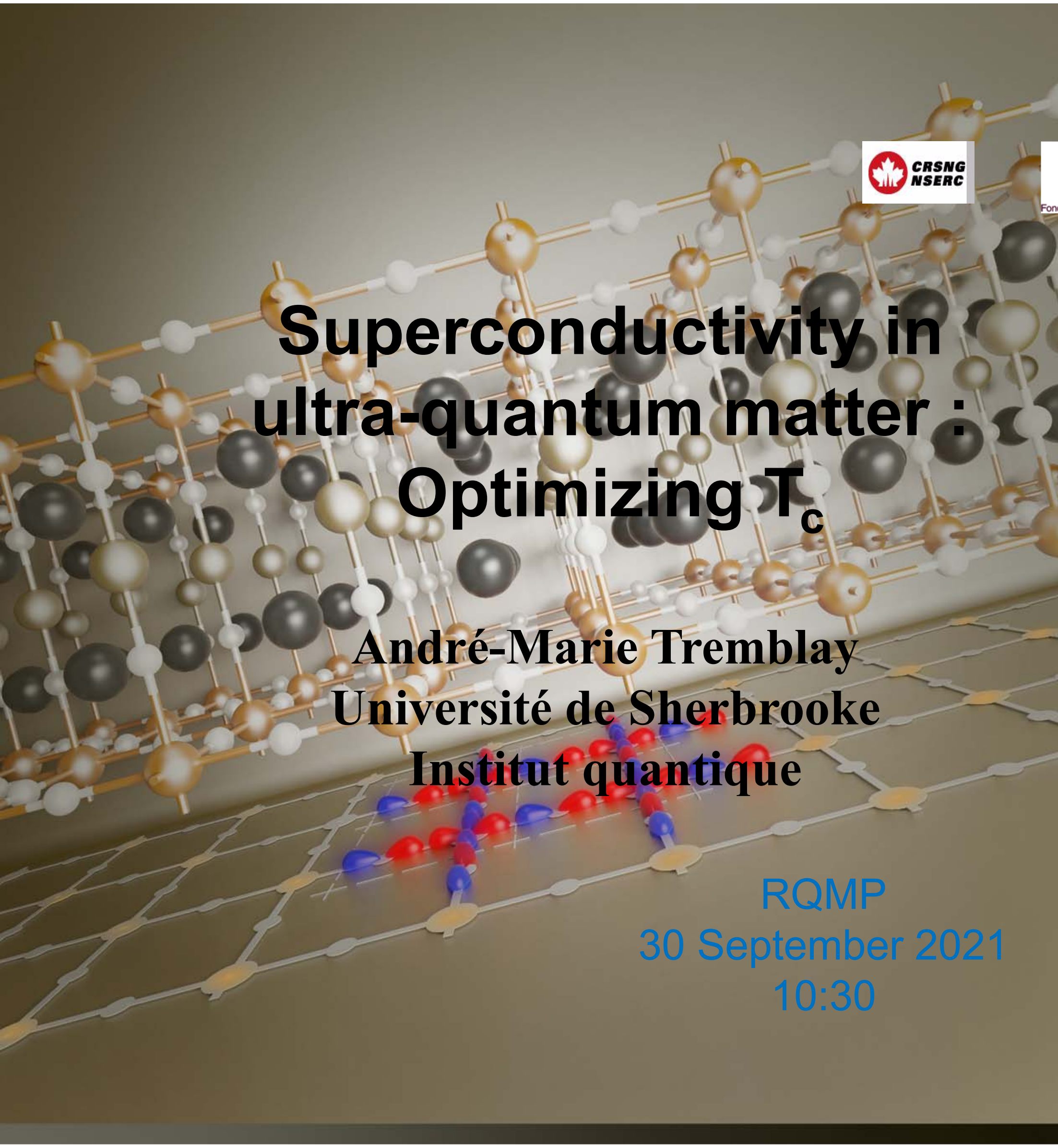
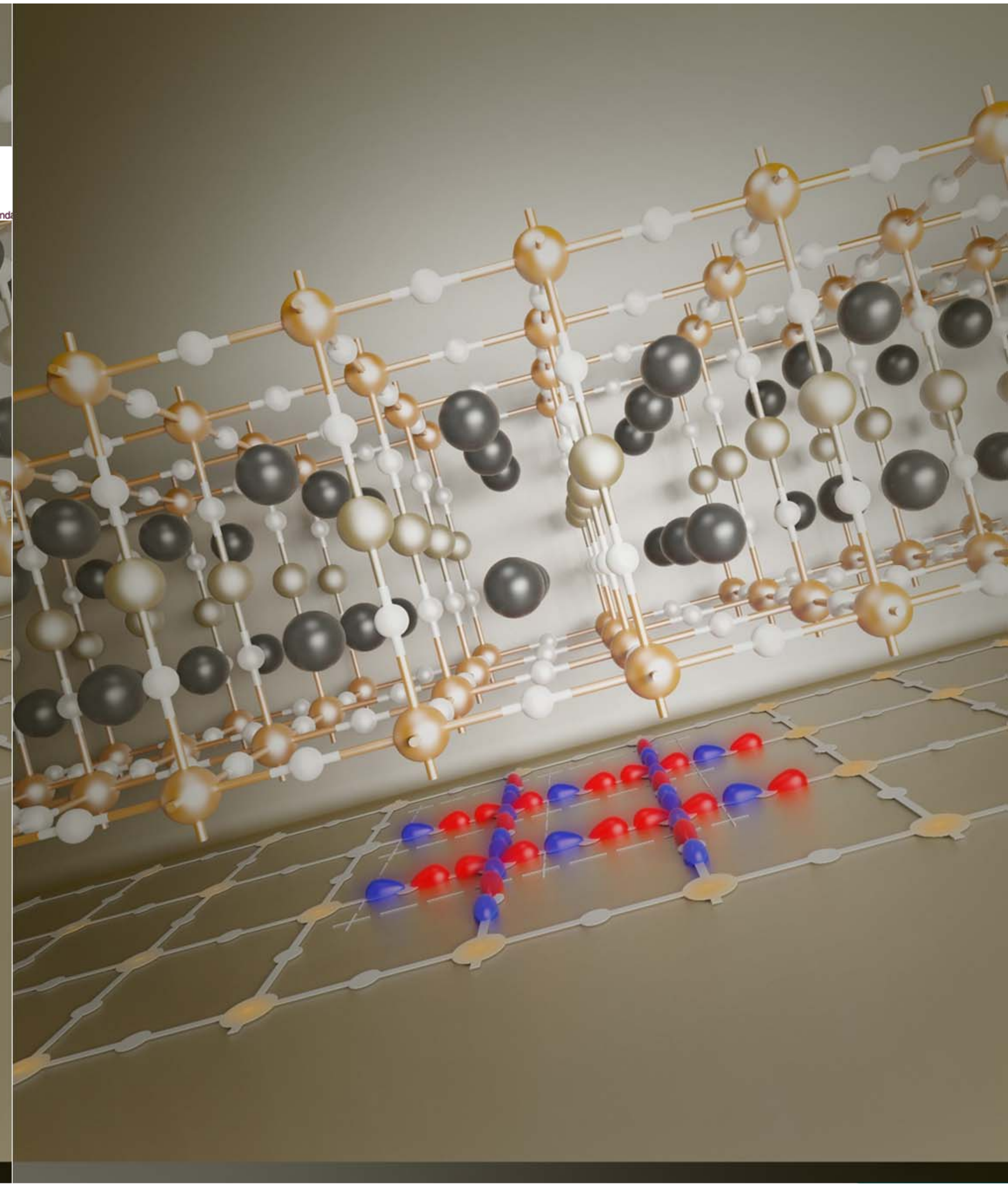


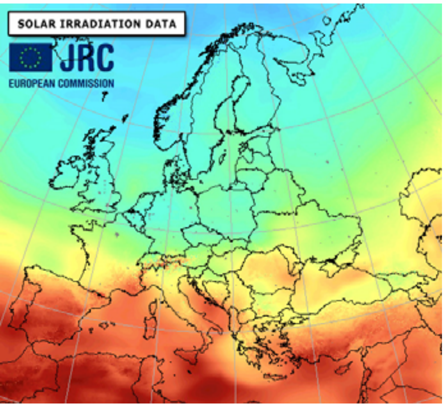
Superconductivity in ultra-quantum matter : Optimizing T_c

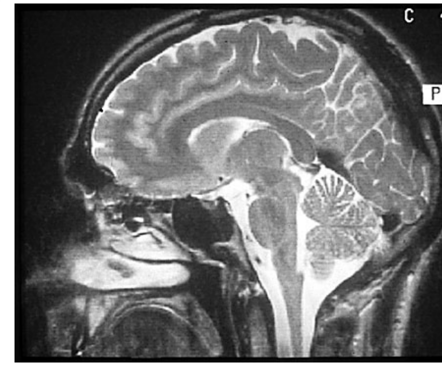
André-Marie Tremblay
Université de Sherbrooke
Institut quantique

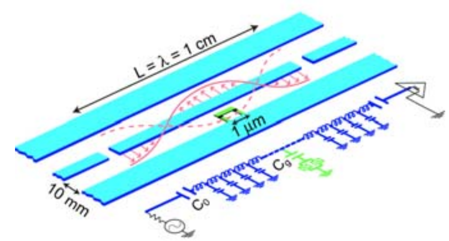
RQMP
30 September 2021
10:30



Applications



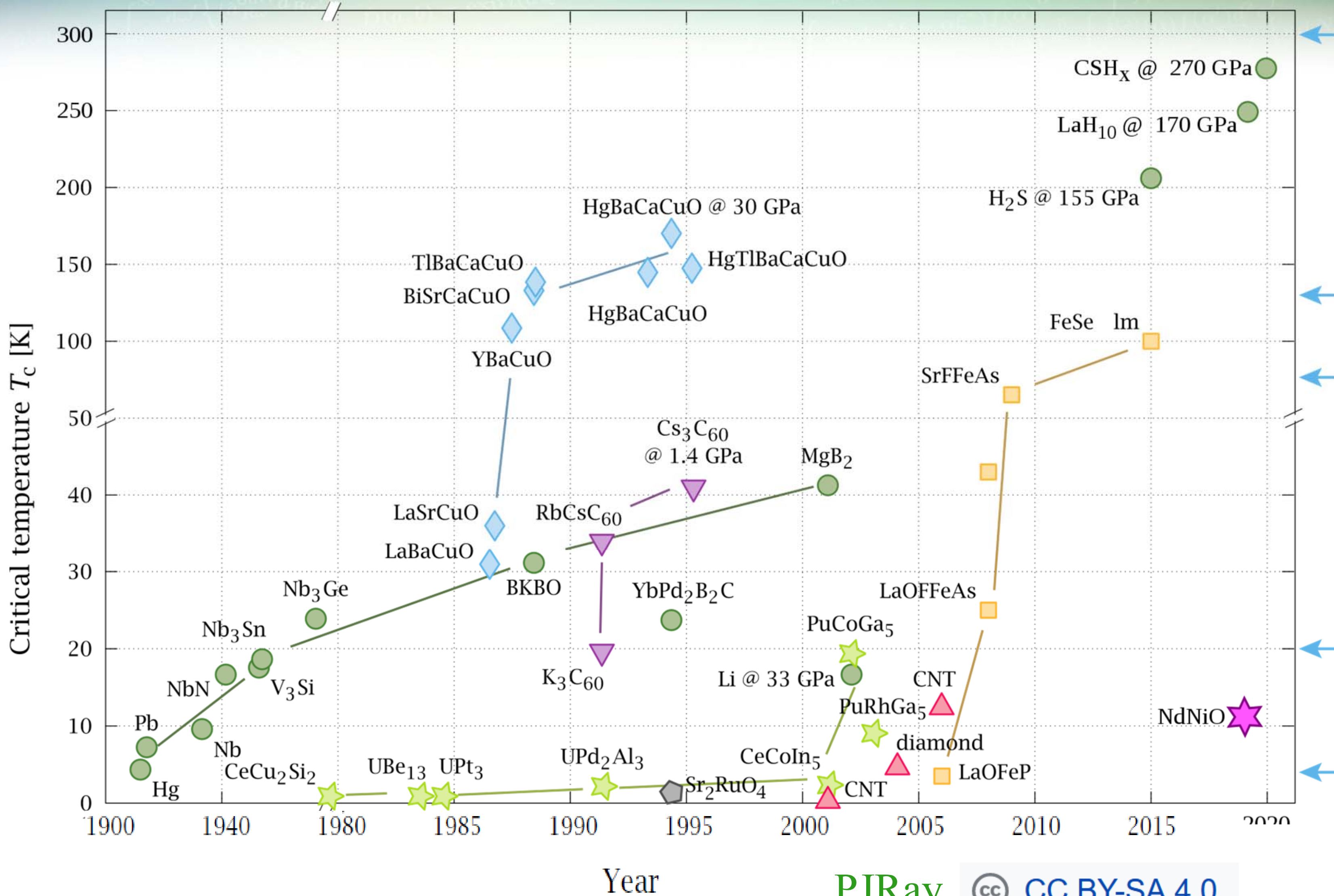




Alexandre Blais, et al. Phys. Rev. A **69**, 062320 (2004)

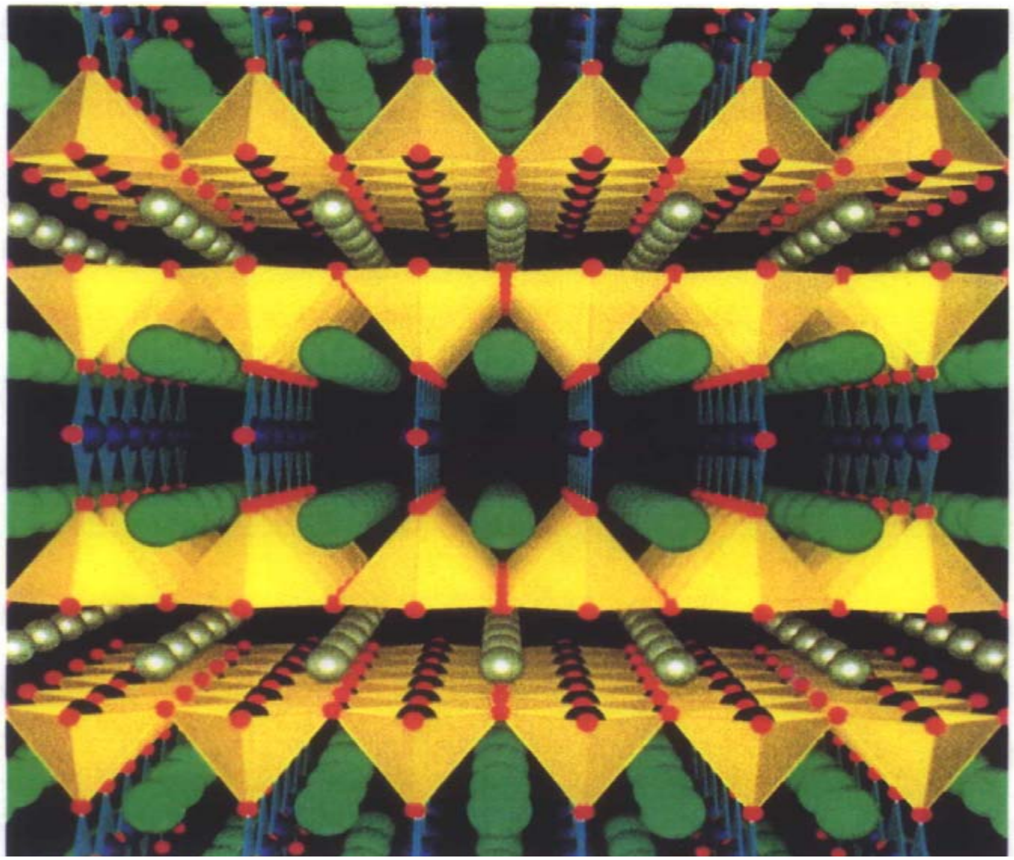
Photo IBM

Can we have superconductivity at room temperature?

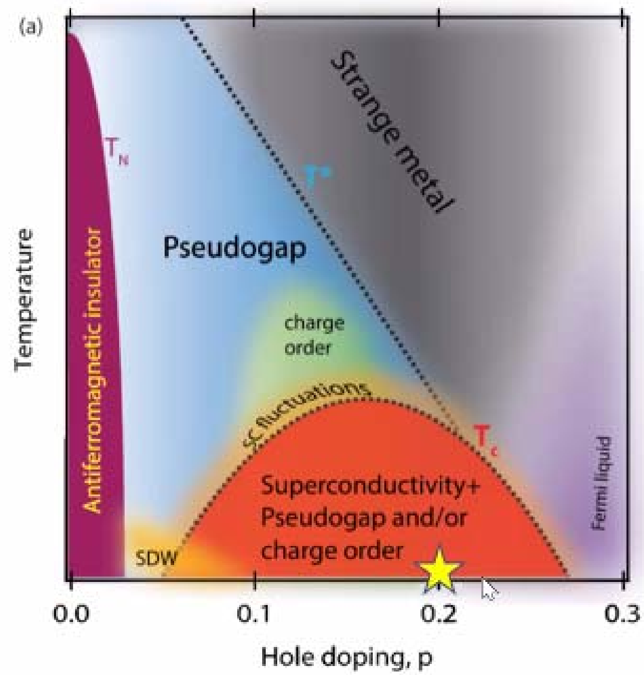


PJRay CC BY-SA 4.0

Cuprates : Atomic structure



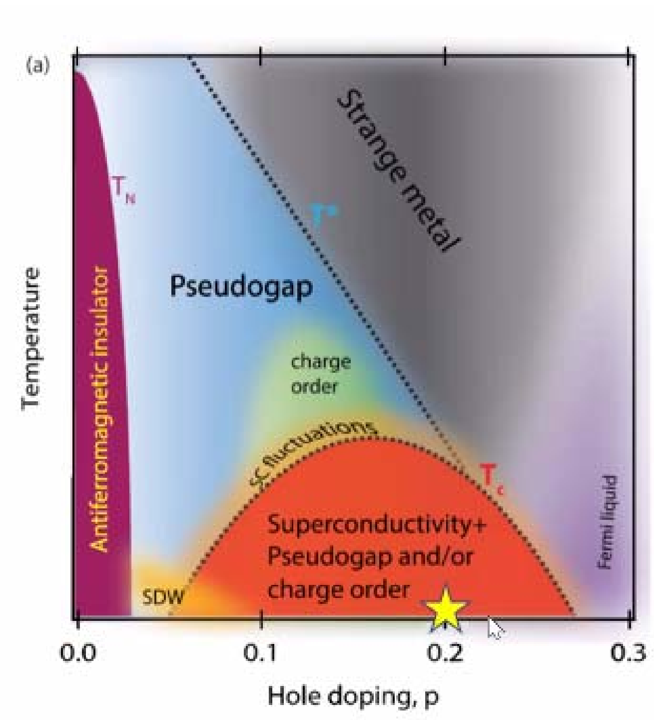
- Who ordered this?



Vishik, Rep. Prog. Phys. (2018)

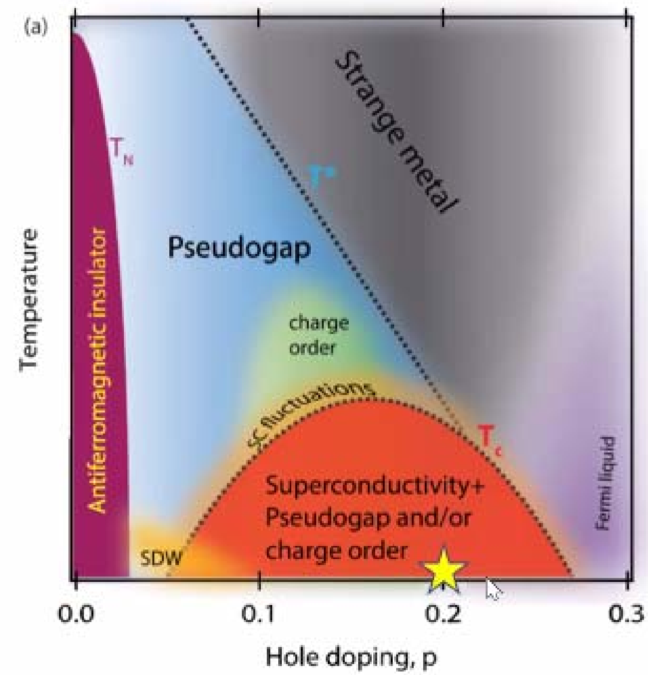
- Mott insulator
- Pseudogap
- Strange metal
- Quantum critical point (QCP)
- Competing ground states
- Superconductivity in the presence of strong repulsion

- 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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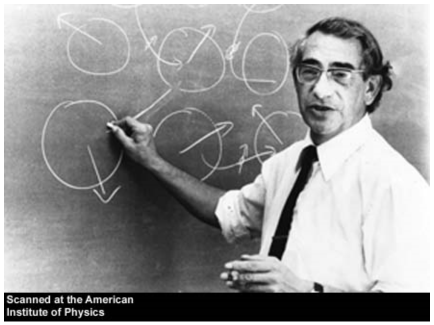
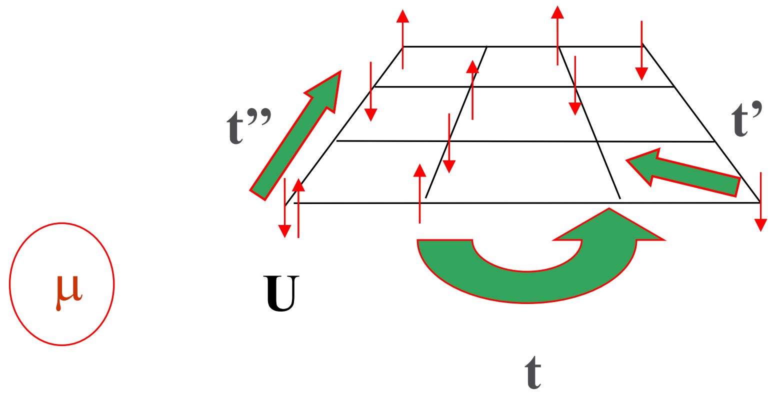
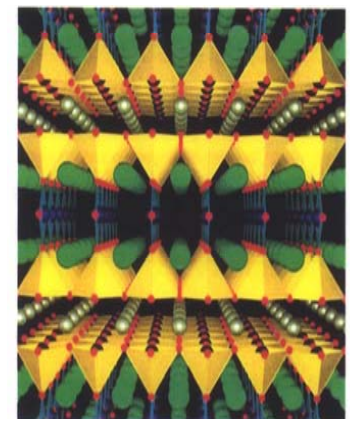
Hubbard model



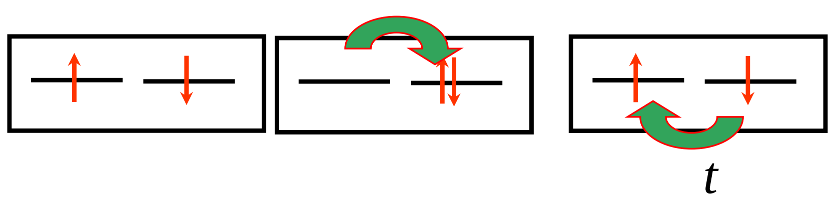


1931-1980



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

Spin 1/2



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

Attn: Charge transfer insulator

Outline

- Method
- One-band Hubbard model
  – d-wave superconductivity
- Three-band Hubbard model : oxygen can probe the details
  – Calculations explain three experiments that show how to optimize d-wave superconductivity

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 repulsion

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

Method :
The precursors

Hohenberg-Kohn : Exchange correlation
Kohn-Sham : Basis set
Density Functional Theory

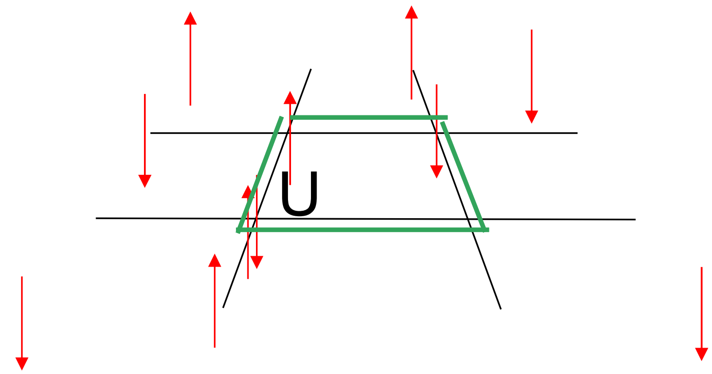
Method

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

Localized



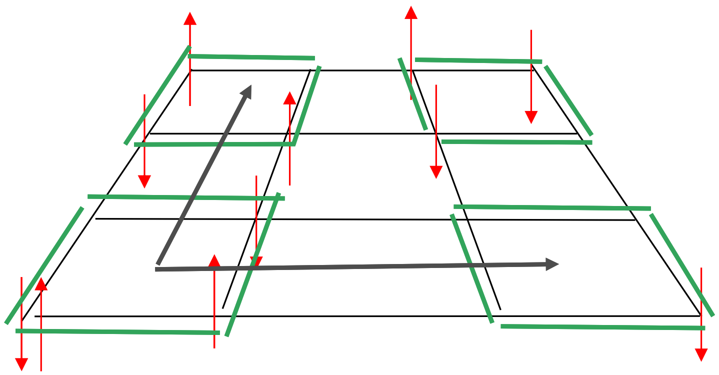
Lichtenstein *et al.*,PRB 2000
Kotliar *et al.*, PRB 2000
M. Potthoff, EJP 2003

REVIEWS
Maier, Jarrell et al., RMP. (2005)
Kotliar *et al.* RMP (2006)
AMST *et al.* LTP (2006)

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

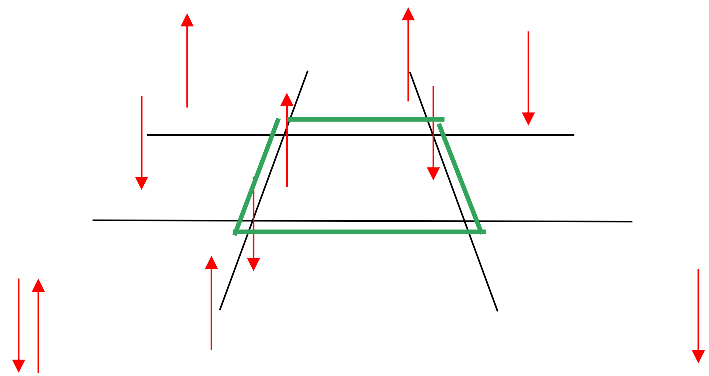
Localized and delocalized pictures C-DMFT

Delocalized



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

Localized

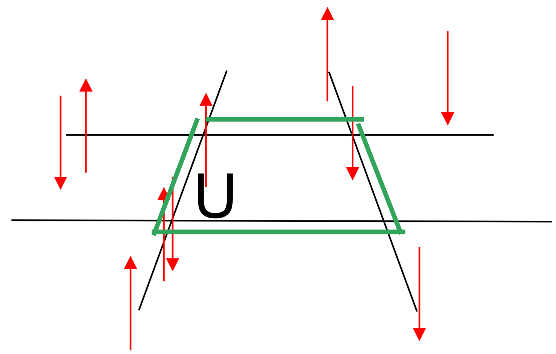


$$G_{ij} = \int \frac{d^d\tilde{k}}{(2\pi)^d} \left(\frac{1}{(i\omega_n+\mu)I-\varepsilon\left(\tilde{k}\right)-\Sigma} \right)_{ij}$$

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

Impurity solvers

Impurity solver (Exact diagonalisation)



Caffarel, Krauth, PRL **72** 1545 (1994)

QCM David Sénéchal

Impurity solver : continuous-time quantum Monte Carlo

$$Z = \int \mathcal{D}[\psi^\dagger, \psi]\, \mathrm{e}^{-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{K}} \psi^\dagger_{\mathbf{K}}(\tau) \Delta_{\mathbf{K}}(\tau,\tau') \psi_{\mathbf{K}}(\tau')}$$

Hybridization expansion :

Werner Millis PRB **74**, 155107 (2006)
Werner Millis B **75**, 085108 (2007)
Haule, PRB **75**, 155113 (2007)
Sémon, Sordi, AMST PRB **89**, 165113 (2014)
Sémon, Yee, Haule, AMST PRB **90,** 075149 (2014)

triqs   **ALPSCore / CT-HYB**   **iQIST**   **ComCTQMC**

Some groups using these methods for cuprates

- Europe:
  - Georges, Parcollet, Ferrero, Civelli (Paris)
  - Lichtenstein, Potthoff, (Hamburg) Aichhorn (Graz), Liebsch (Jülich) de Medici (Grenoble) Capone (Italy)
- USA:
  - Gull (Michigan) Millis (Columbia)
  - Kotliar, Haule (Rutgers) (Haule, Kotliar PRB **76**, 104509 (2007))
  - Jarrell (Louisiana)
  - Maier, Okamoto (Oakridge)
- Japan
  - Imada (Tokyo) Sakai, Tsunetsugu, Motome
- China
  - Wei Wu …

Critique

+ and -

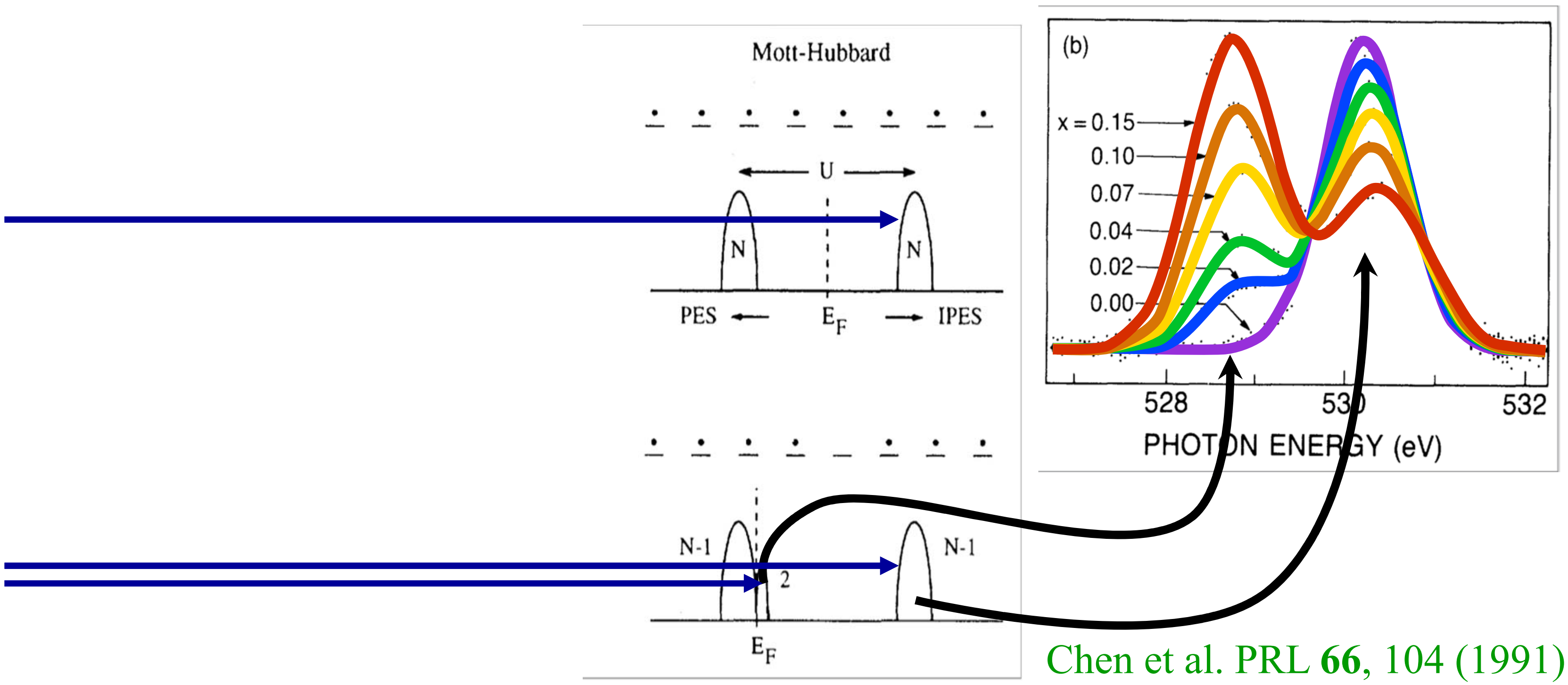
- Long range order:
  - No mean-field factorization on the cluster
  - Symmetry breaking allowed in the bath
- Included exactly:
  - Short-range dynamical and spatial correlations

- Missing:
  - Long wavelength p-h and p-p fluctuations
  - Hence good when the corresponding correlation lengths are small

Cuprates as doped Mott insulators

Mott Insulator : X-Ray absorption

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

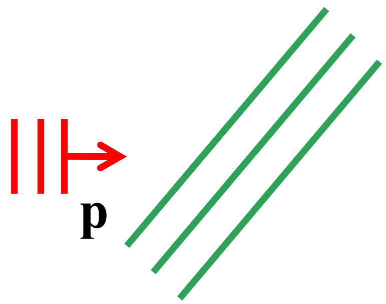


Chen et al. PRL **66**, 104 (1991)

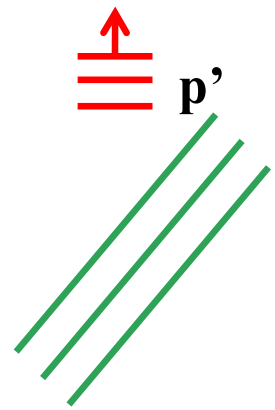
d-wave superconductivity One band model

Superconductivity

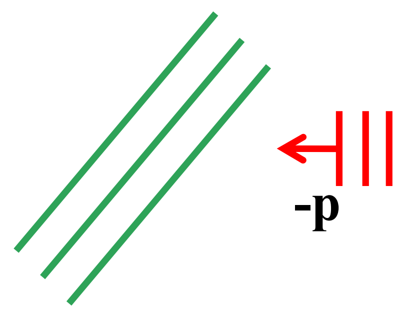
Attraction mechanism in the metallic state



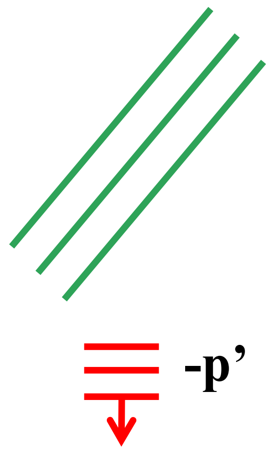
Attraction mechanism in the metallic state



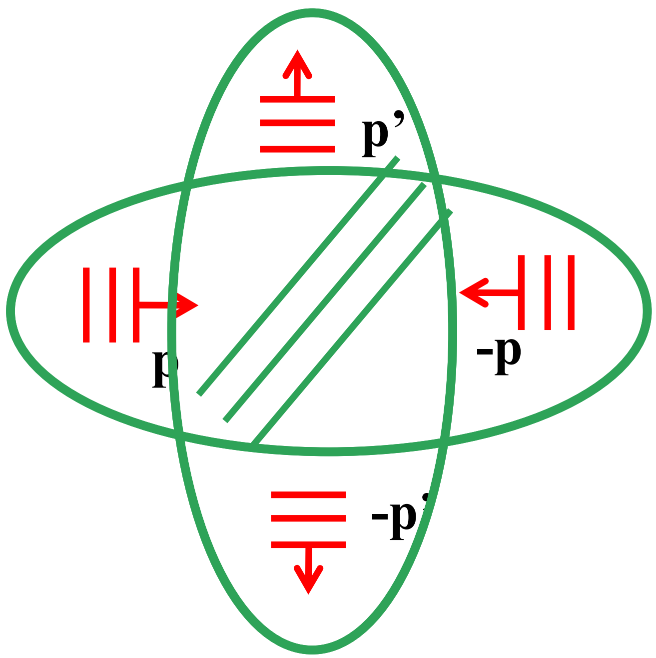
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



#1 Cooper pair, #2 Phase coherence

$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow}$$

$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \left\langle \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} \right\rangle \left\langle \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \right\rangle$$

$$|\mathrm{BCS}(\theta)\rangle = \ldots + e^{iN\theta}|N\rangle + e^{i(N+2)\theta}|N+2\rangle + \ldots.$$

The weak-correlation limit : Boson exchange

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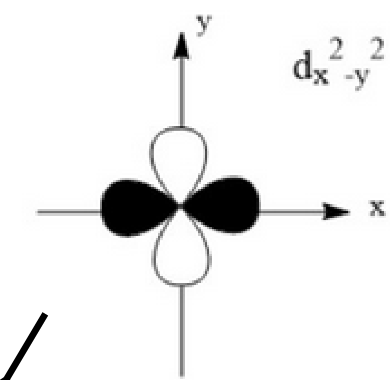
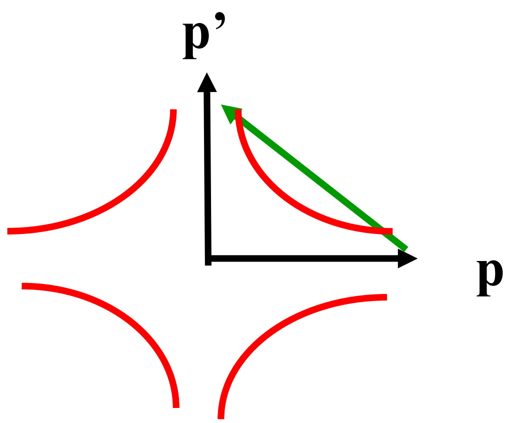
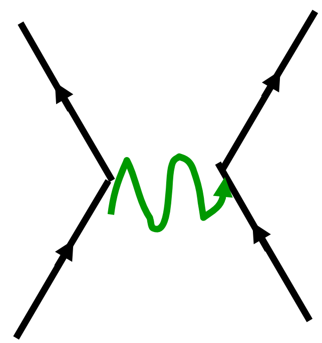
Cartoon « BCS » weak-coupling picture



$$\Delta_{\mathbf{p}} = -\frac{1}{2V}\sum_{\mathbf{p}'} U(\mathbf{p}-\mathbf{p}')\frac{\Delta_{\mathbf{p}'}}{E_{\mathbf{p}'}}\left(1-2n\left(E_{\mathbf{p}'}\right)\right)$$





Béal–Monod, Bourbonnais, Emery
P.R. B. **34**, 7716 (1986).
D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch
P.R. B **34**, 8190-8192 (1986).
Kohn, Luttinger, P.R.L. **15**, 524 (1965).

Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

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

The strong-correlation limit : Superexchange

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A cartoon strong correlation picture

$$\hat{\mathcal{H}}_{mod\grave{e}le\ t-J} = -t \sum_{\langle i,j \rangle\ \sigma} \hat{P}\left(\hat{c}^\dagger_{i\sigma}\hat{c}_{j\sigma} + c.h\right)\hat{P} + J\sum_{\langle i,j \rangle}\left(\hat{\vec{S}}_i.\hat{\vec{S}}_j - \frac{1}{4}\hat{n}_i\hat{n}_j\right)$$

$$\begin{aligned}
J\hat{S}^z_i\hat{S}^z_j &= J(\hat{n}_{i\uparrow} - \hat{n}_{i\downarrow})(\hat{n}_{j\uparrow} - \hat{n}_{j\downarrow}) \\
&= J(\hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow} - \hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow})(\hat{c}^\dagger_{j\uparrow}\hat{c}_{j\uparrow} - \hat{c}^\dagger_{j\downarrow}\hat{c}_{j\downarrow}) \\
&= -J(\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}\hat{c}^\dagger_{j\uparrow}\hat{c}_{j\uparrow} + \hat{c}^\dagger_{i\uparrow}\hat{c}_{i\uparrow}\hat{c}^\dagger_{j\downarrow}\hat{c}_{j\downarrow}) + \ldots \\
&= -J(\hat{c}^\dagger_{j\uparrow}\hat{c}^\dagger_{i\downarrow}\hat{c}_{i\downarrow}\hat{c}_{j\uparrow} + \hat{c}^\dagger_{i\uparrow}\hat{c}^\dagger_{j\downarrow}\hat{c}_{j\downarrow}\hat{c}_{i\uparrow}) + \ldots
\end{aligned}$$

Hartree-Fock :

$$d^* = \langle \hat{c}^\dagger_{j\uparrow}\hat{c}^\dagger_{i\downarrow}\rangle_{\mathcal{H}_{mod\grave{e}le\ t-J}}$$

$$\langle J\hat{S}^z_i\hat{S}^z_j\rangle = -2J\,d^*d + \ldots$$

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

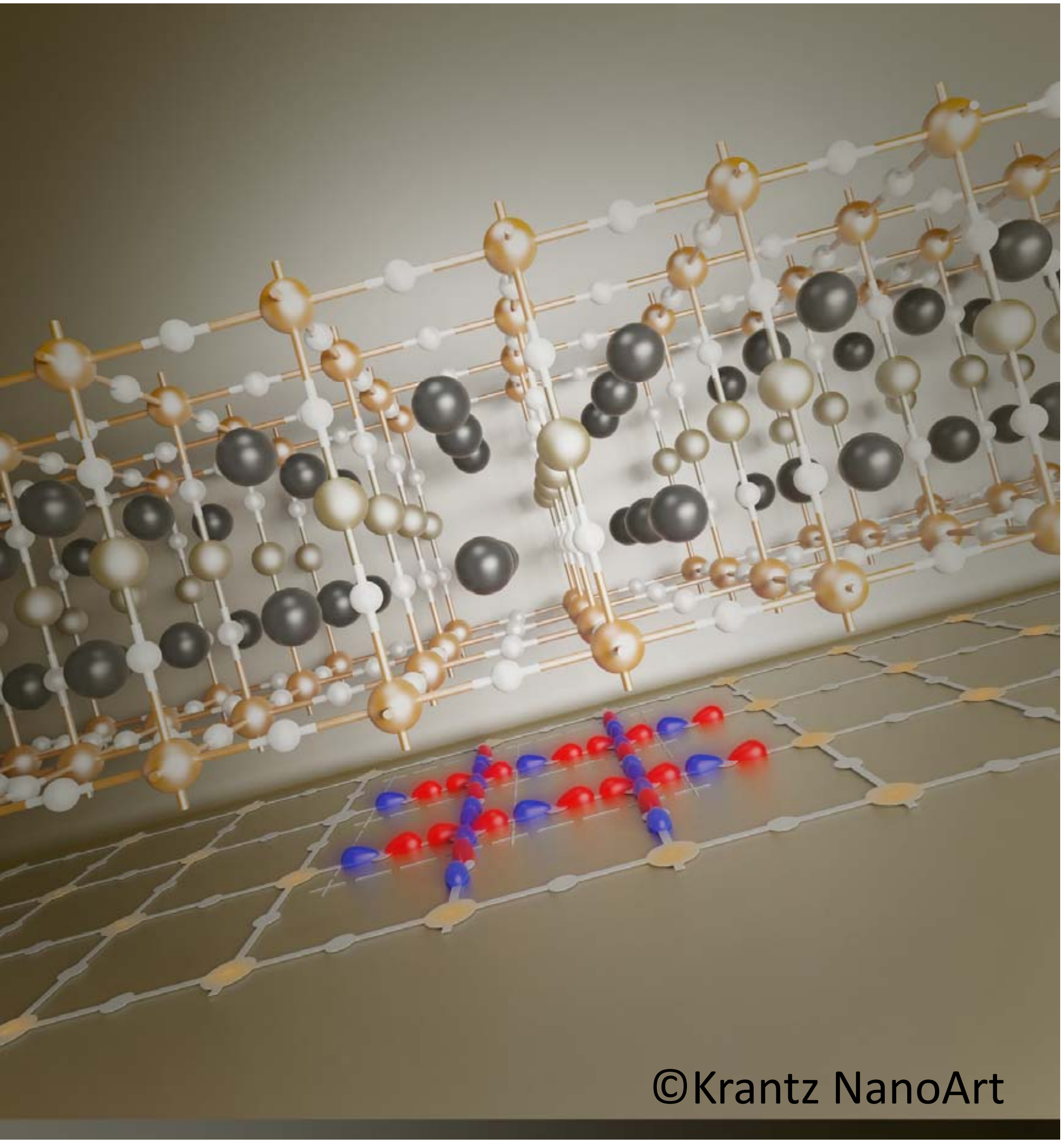
Summary of what we learn from one band d-wave

- Lots of singlets near half-filling

- Superconductivity strongest when kinetic and potential energy are comparable (Scales like J at large U)

- Condensation energy when strong correlations : (confirmed by experiment)
  - From kinetic energy near half-filling
  - From potential energy at large doping

- Phase fluctuations important for the shape of the d-wave dome



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Three-band (Emery VSA) Hubbard model

Sidhartha Dash

Nicolas Kowalski

Patrick Sémon

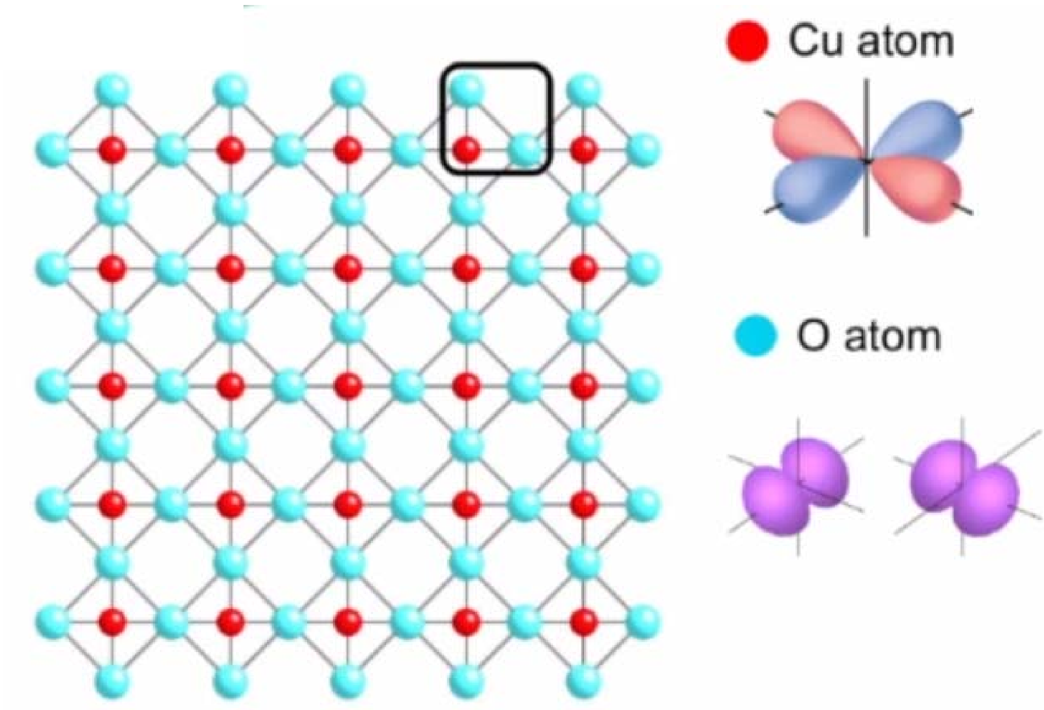
David Sénéchal

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

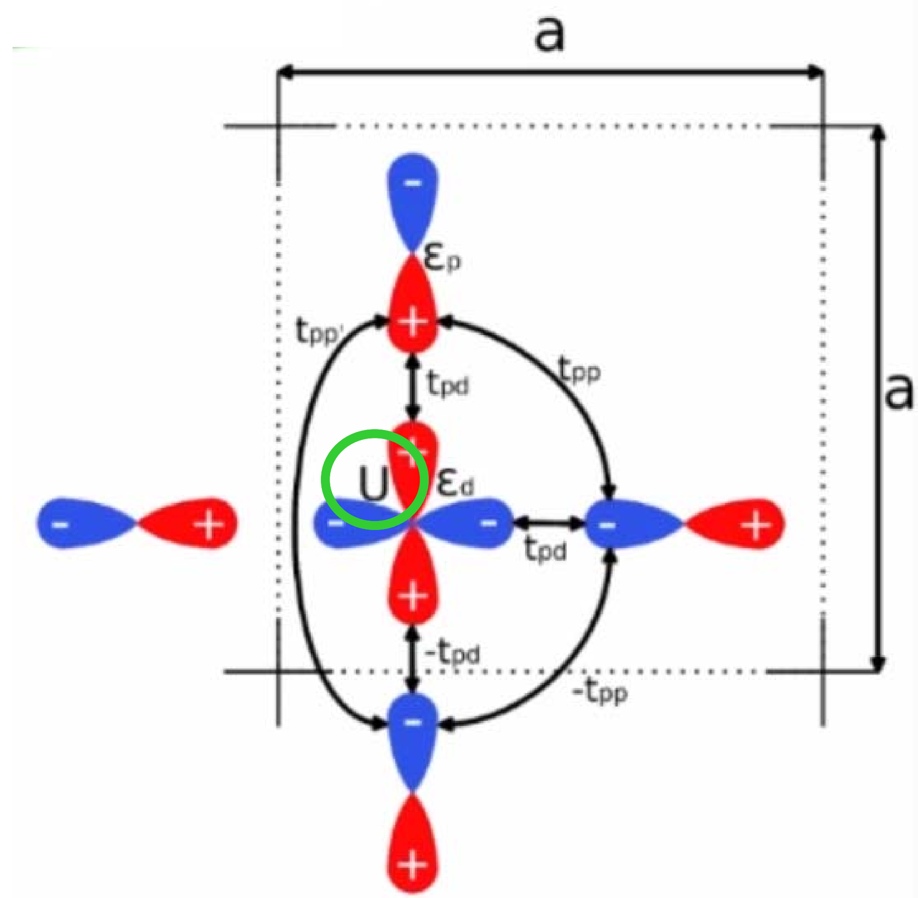
C. M. Varma, S. Schmitt-Rink, and E. Abrahams, Solid State Communications **62**, 681–685 (1987), ISSN 0038-1098,

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

Copper and oxygen planes

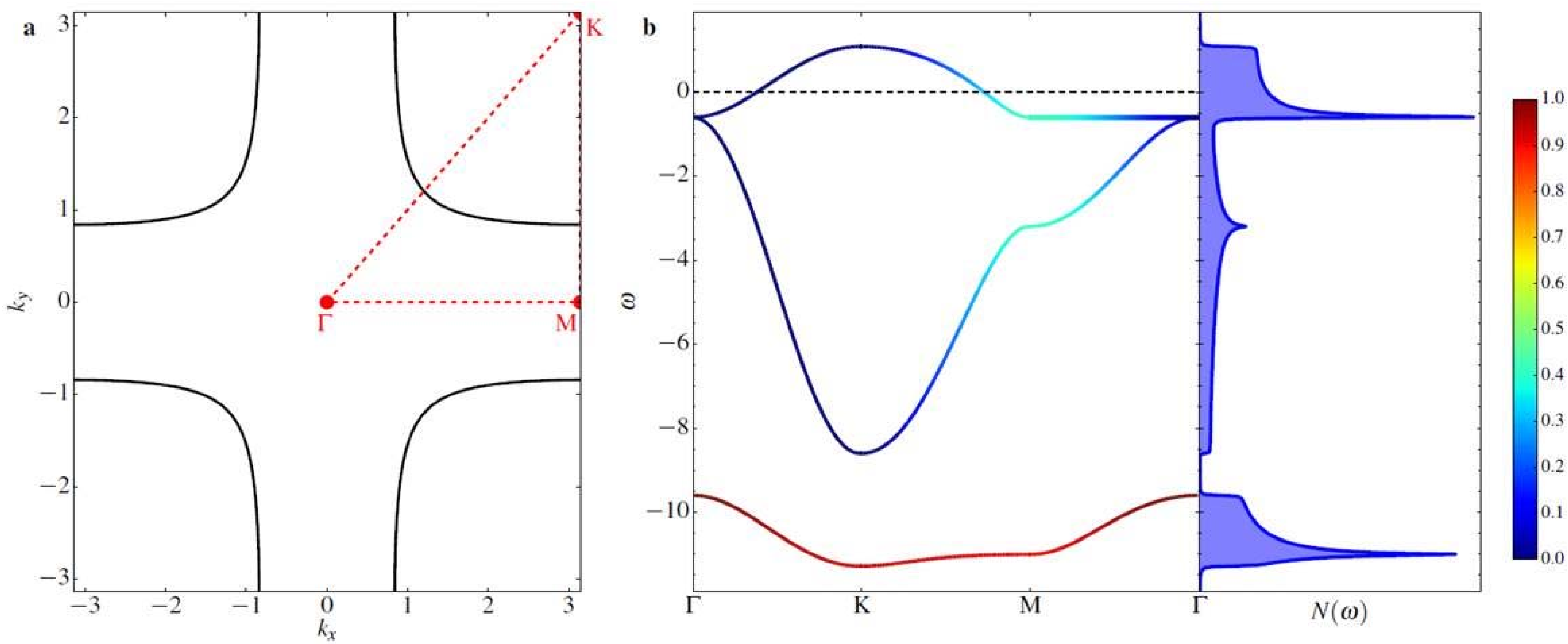


© Nicolas Kowalski



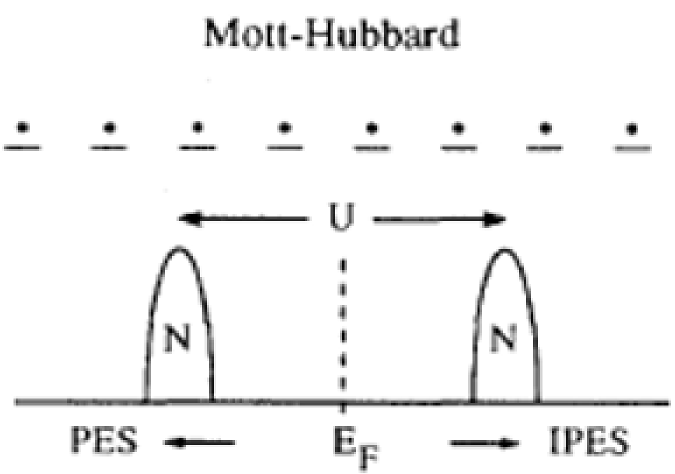
© Nicolas Kowalski

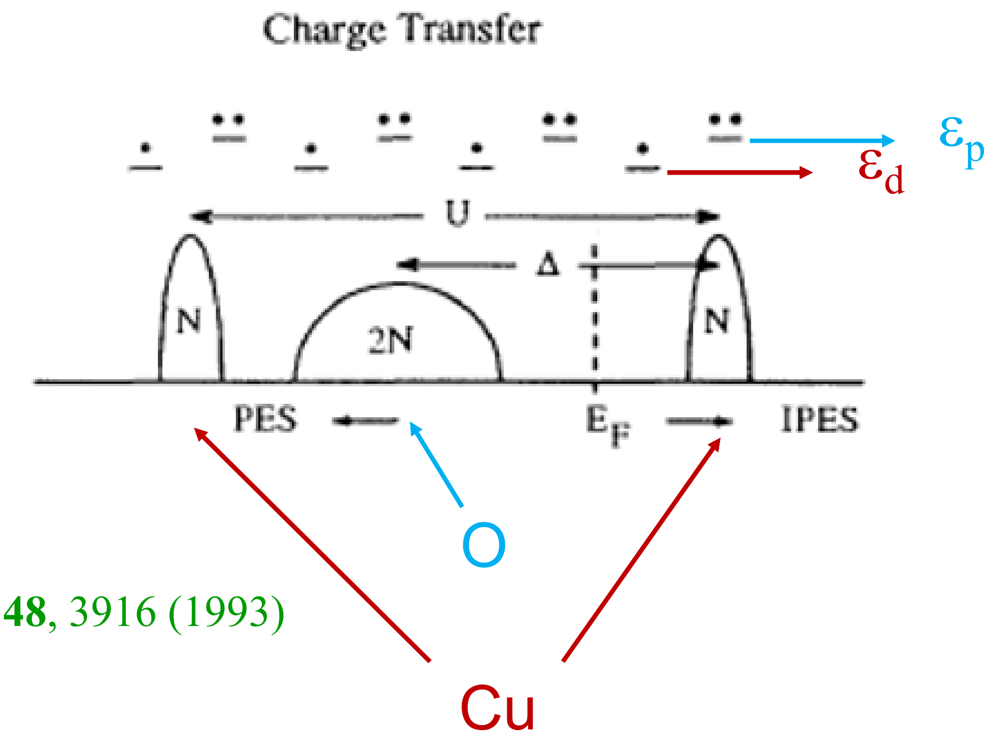
Bands : Copper-Oxygen hybridization



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

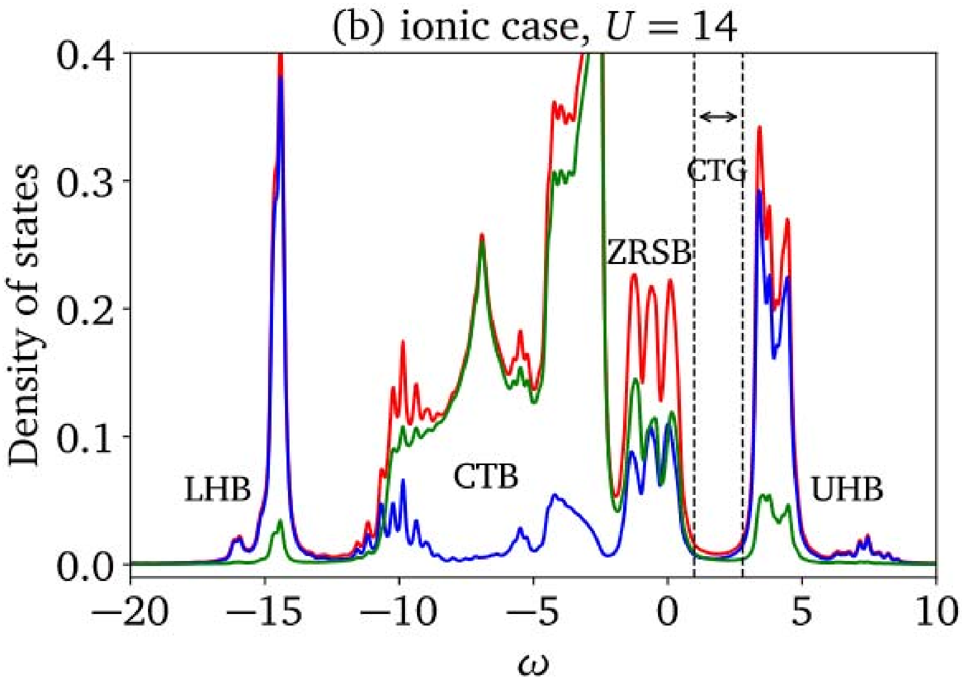
Interactions : Charge-transfer insulator

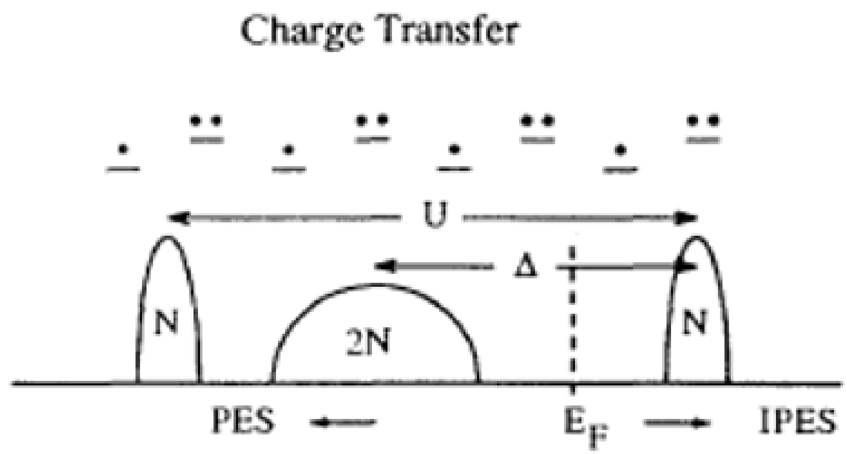


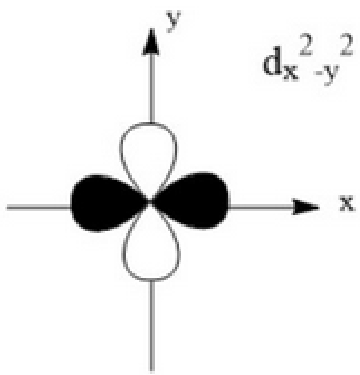


Meinders *et al*. PRB **48**, 3916 (1993)

"Ionic" limiting cases with manageable sign problem



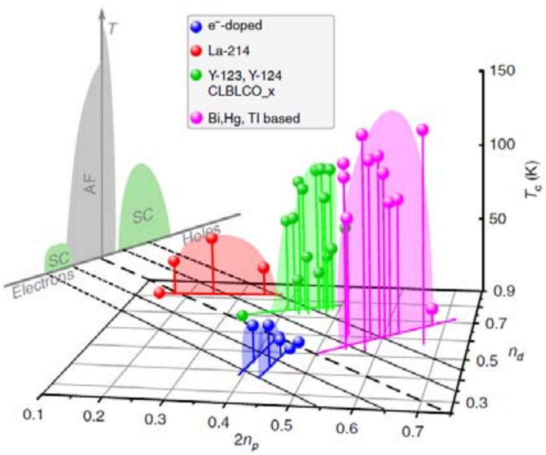




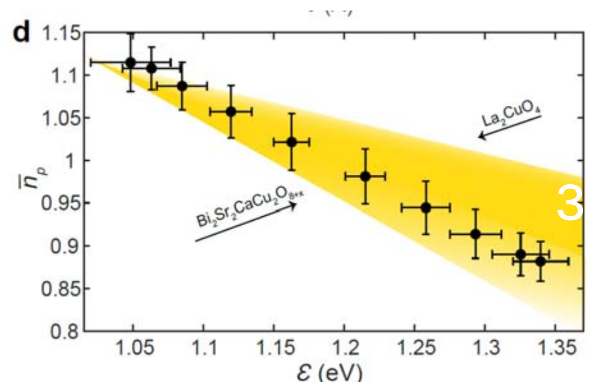
d-wave Superconductivity

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

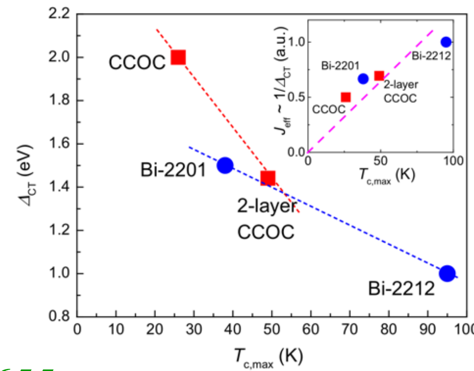
Three experimental observations on optimizing T_c



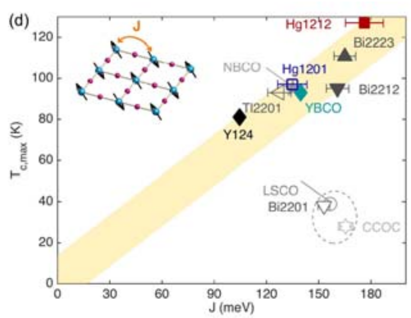
Rybicki, … Haase,
Nat. Comm. 7, 11413
(2016)



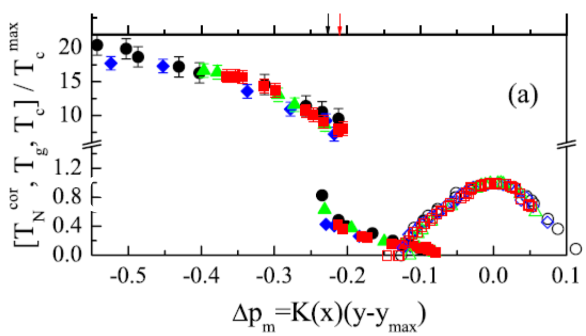
O'Mahony *et al.* arXiv:2108.03655



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



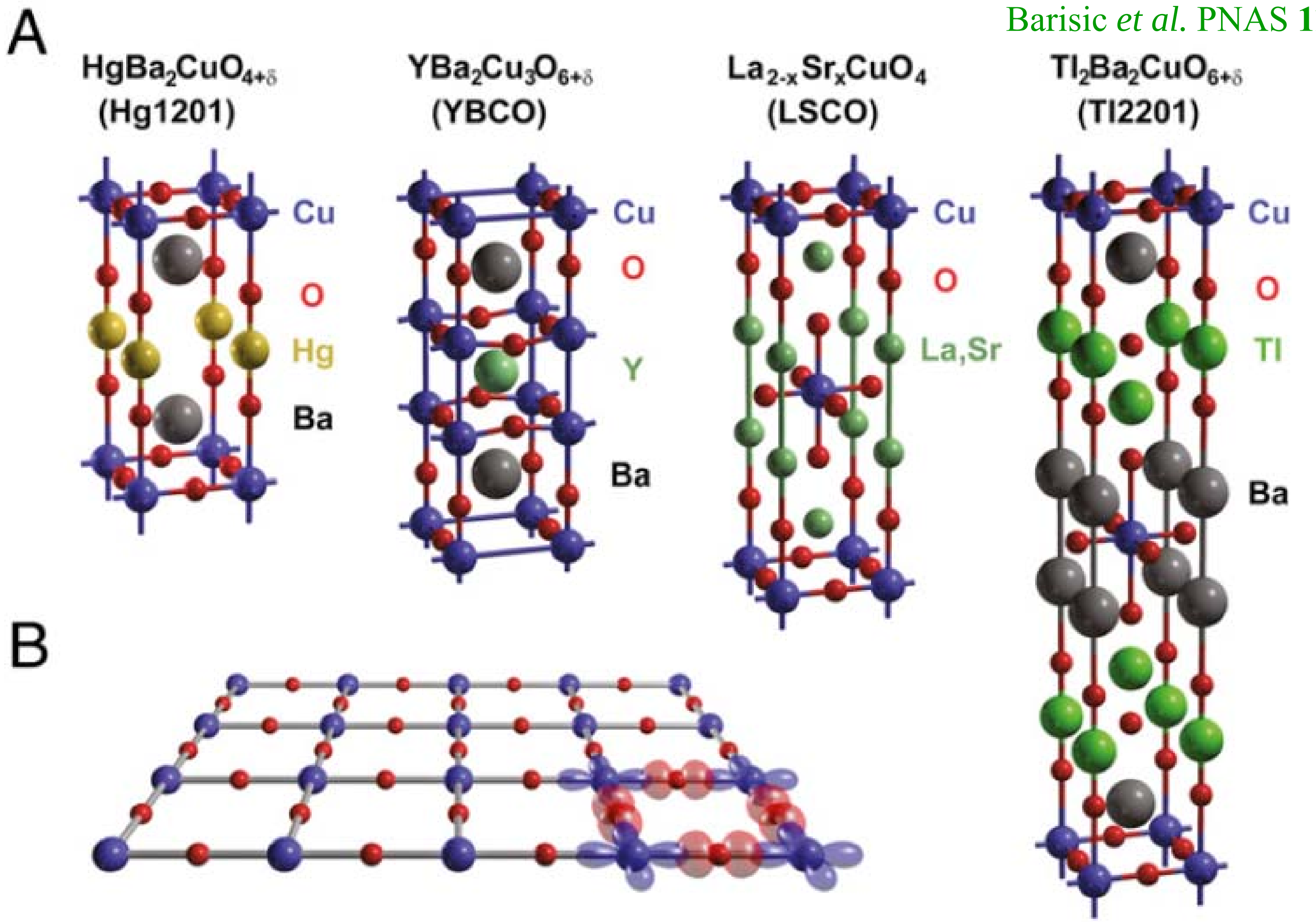
Lichen Wang, *et al.*
arXiv 2011.05029



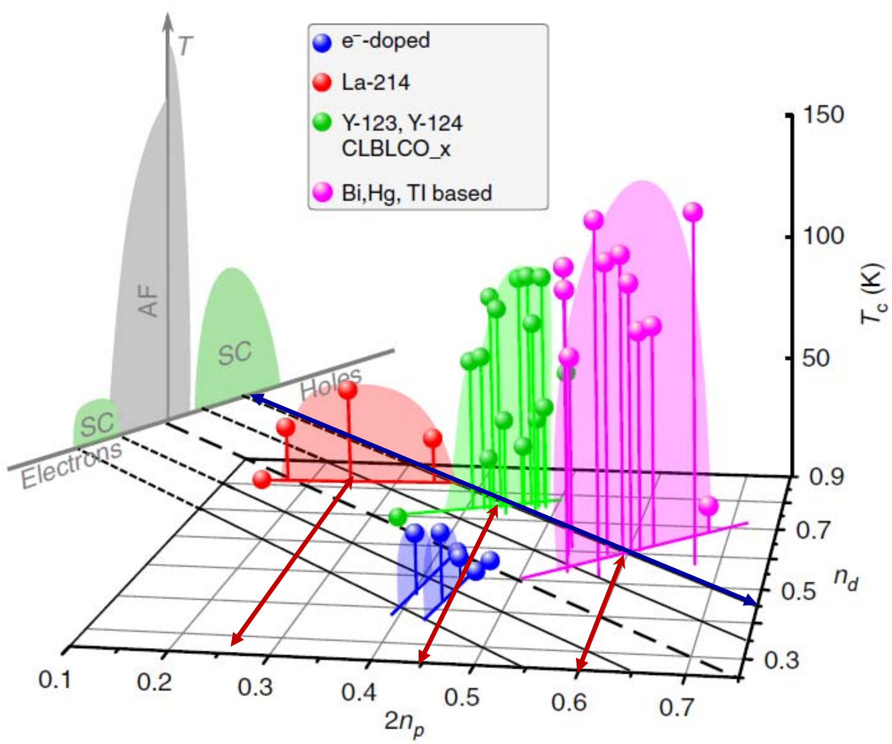
A. Keren New J. Phys. **11** 065006

There are different kinds of cuprates : All with CuO_2 planes

Barisic *et al*. PNAS **110**, 12235 (2013)



#1 Optimizing T_c with oxygen hole content

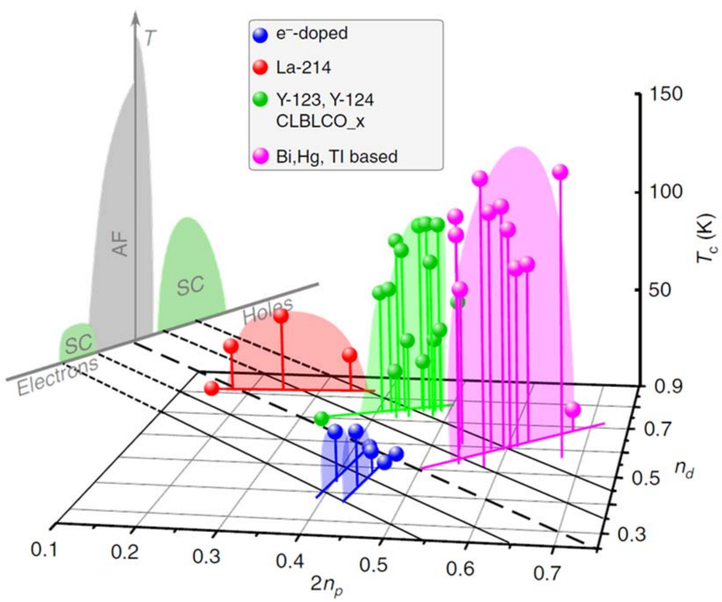


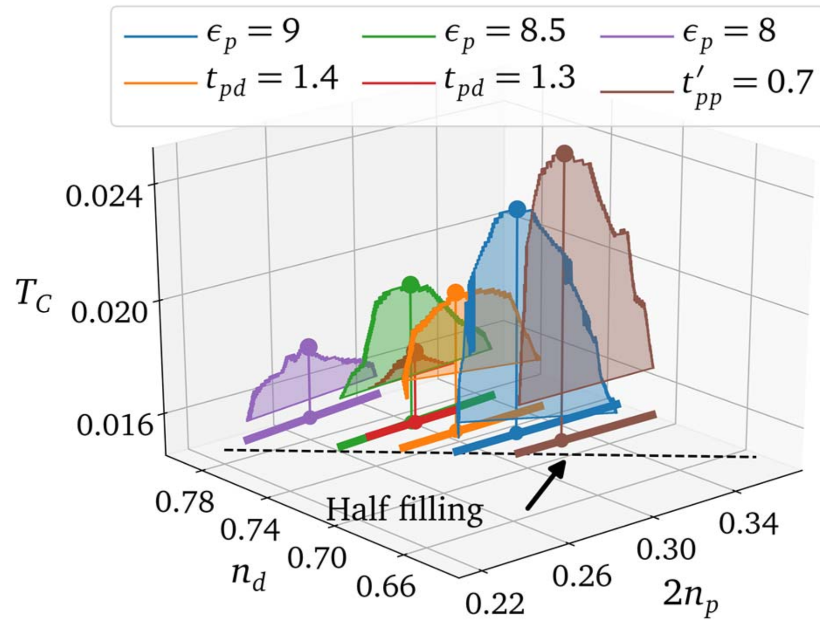
Rybicki,,, Haase, Nat. Comm. 7, 11413 (2016)

Results

Critical Temperature

- $\varepsilon_p - \varepsilon_d = 7.0$, $t_{pd} = 1.5$, $t_{pp} = 1.0$, $t'_{pp} = 1.0$





D. Rybicki et al. "Perspective on the phase diagram of cuprate high-temperature superconductors," Nature Communications, vol. 7, p. 11413, 2016

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

More realistic models

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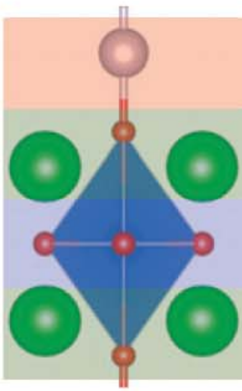
Optimizing T_c

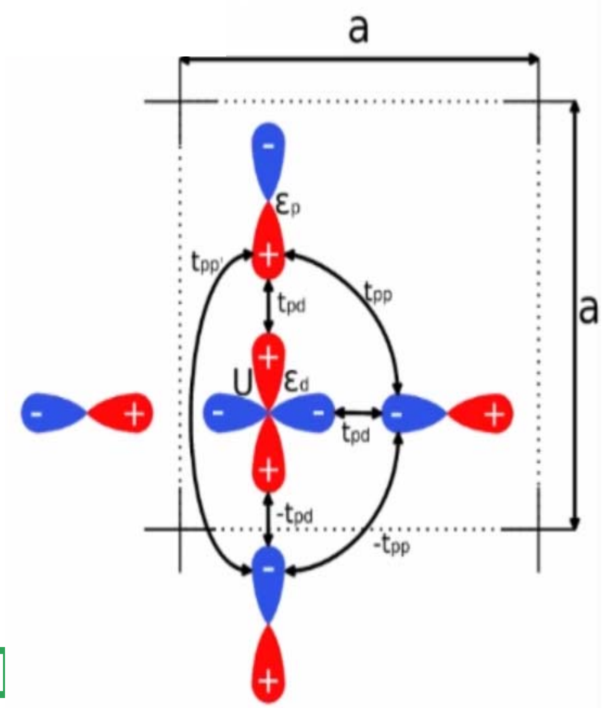


	charge	dopants	structure	hamiltonian
HgO_δ	balances -2 charge	supplies	harbors dopants	tunes chemical potential
BaO	neutral	inert	protects CuO_2 from disorder	tunes in-plane t, t', U
CuO_2	-2 charge/u.c.	accepts	roughly sets lattice const.	superconducts
BaO			(same as other CaS layer)	

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

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



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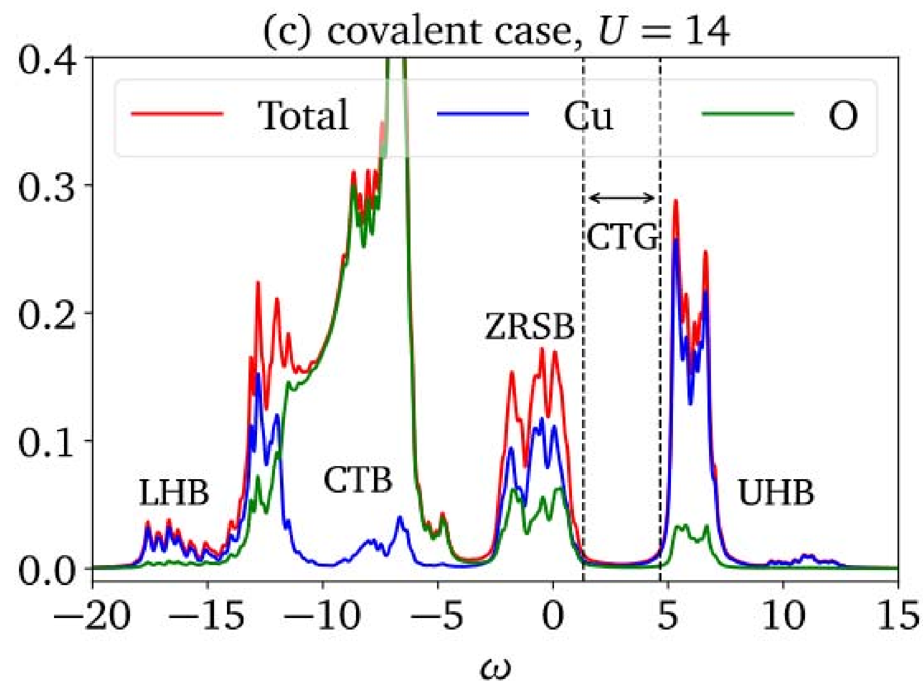
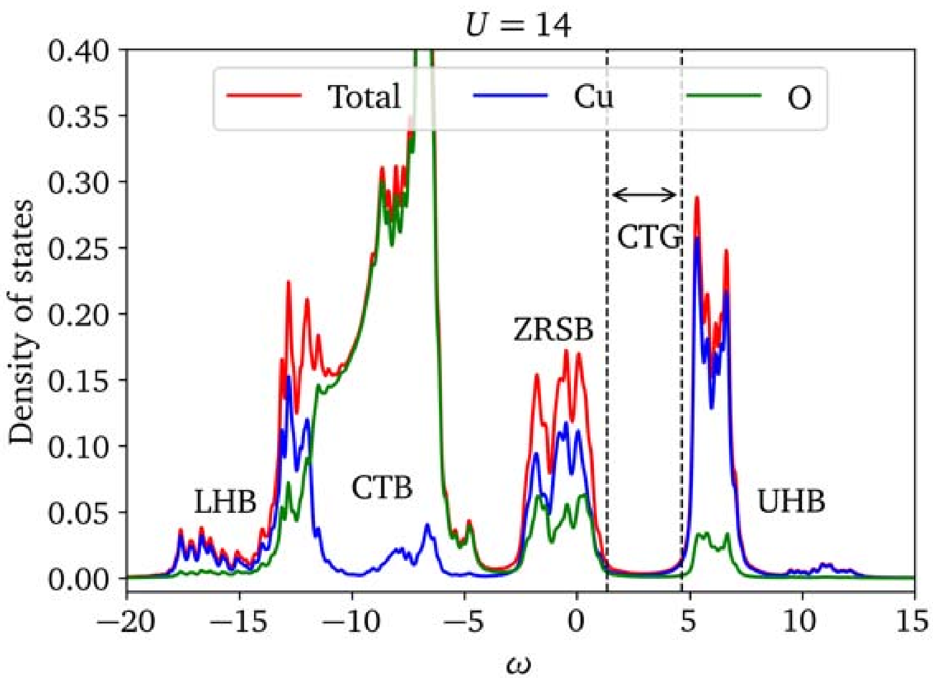
Weber, Yee, Haule, Kotliar, EPL 100, 2012

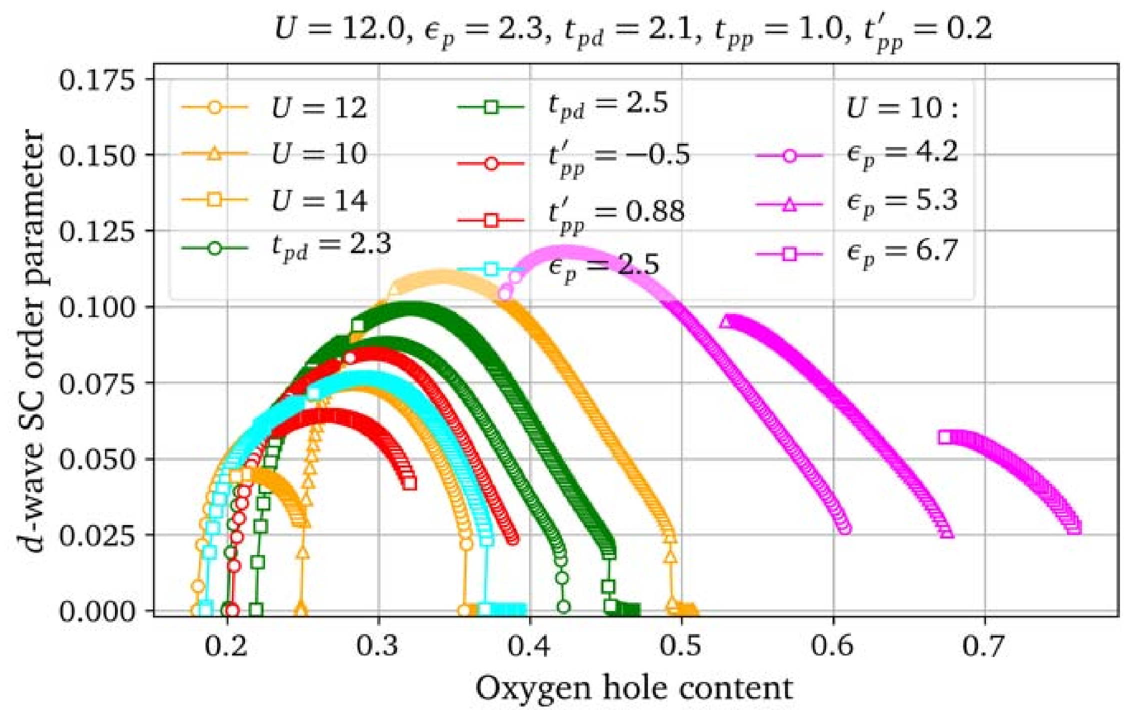
Density of states



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

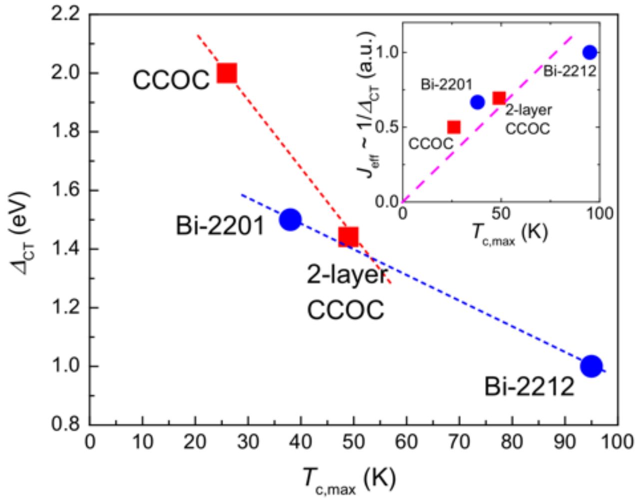
T = 0 superconducting domes for the covalent model



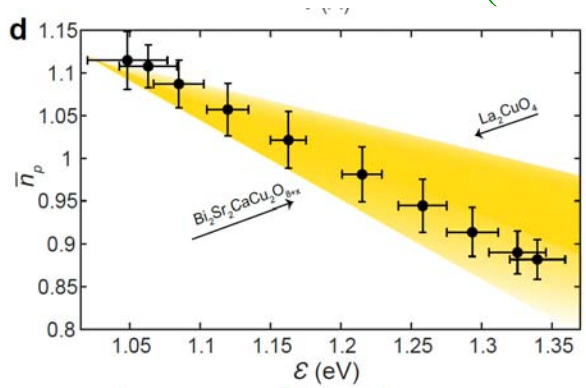


Kowalski, Dash, Sémon, Sénéchal, A-M.T.
PNAS **118** (40) e2106476118 (2021)

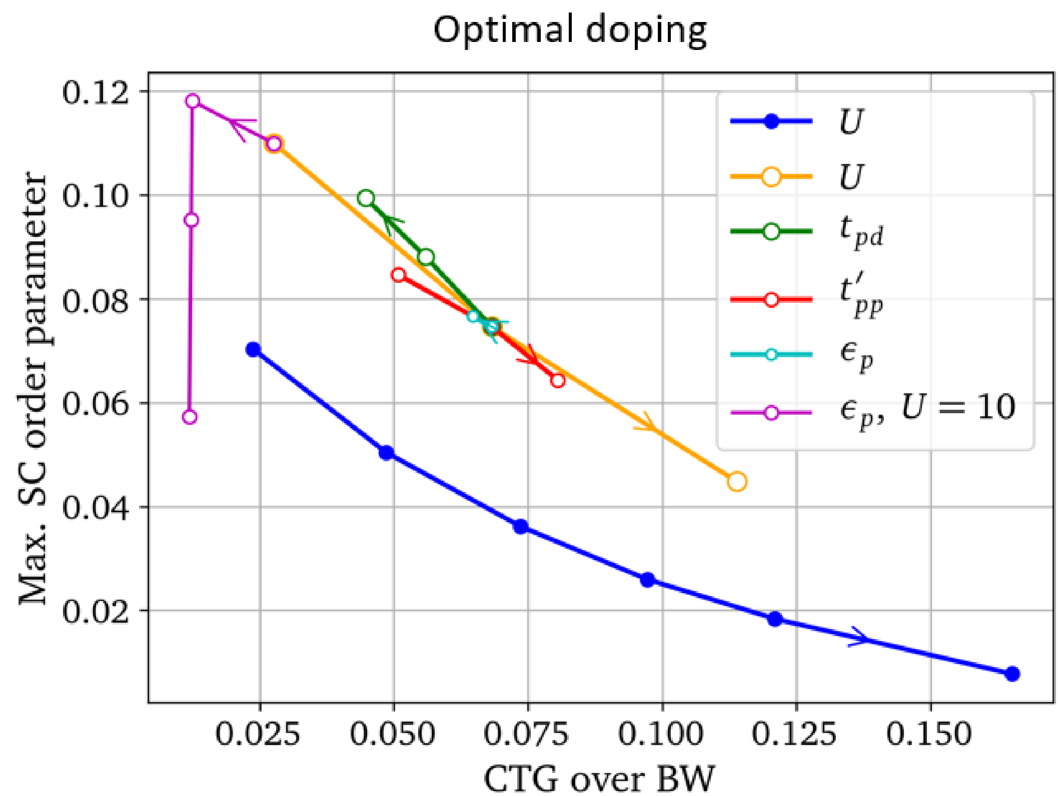
#2 Optimizing T_c with CT gap Δ (Oxygen as a witness)



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

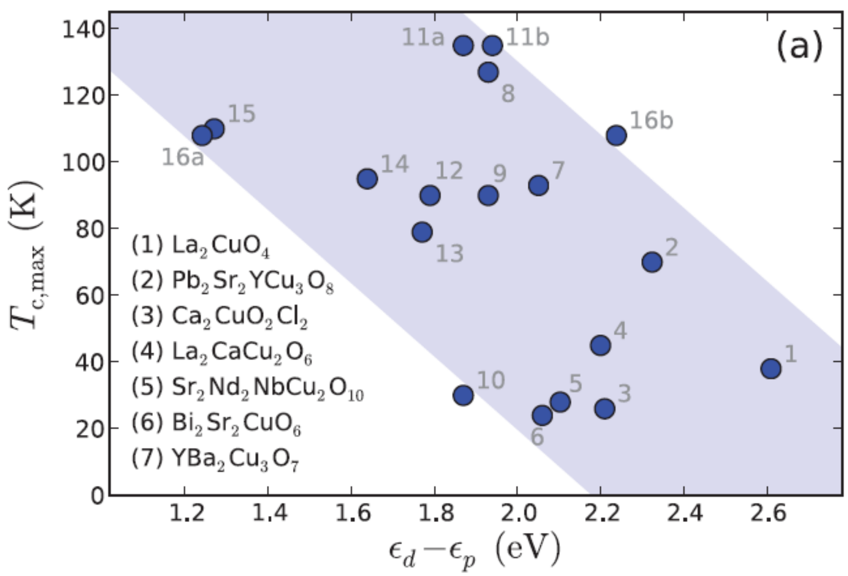


O'Mahony *et al.* arXiv:2108.03655

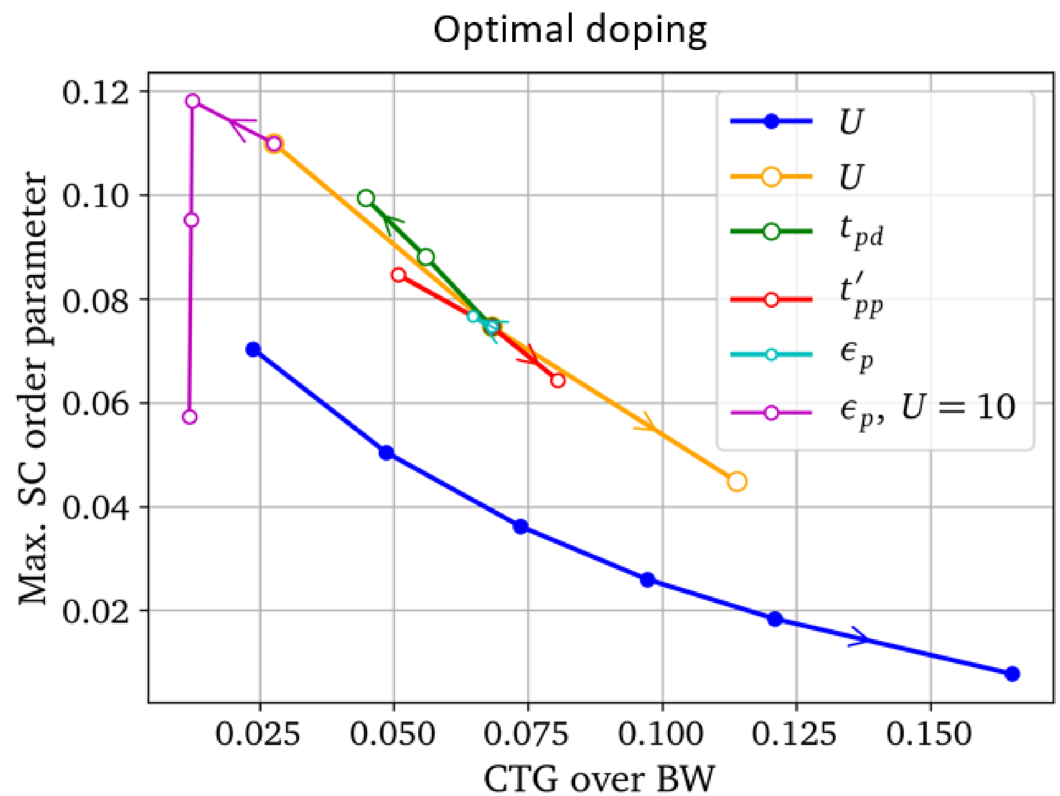


Kowalski, Dash, Sémon, Sénéchal, A-M.T.
PNAS **118** (40) e2106476118 (2021)

Experimental puzzle #2 with Charge Transfer Gap

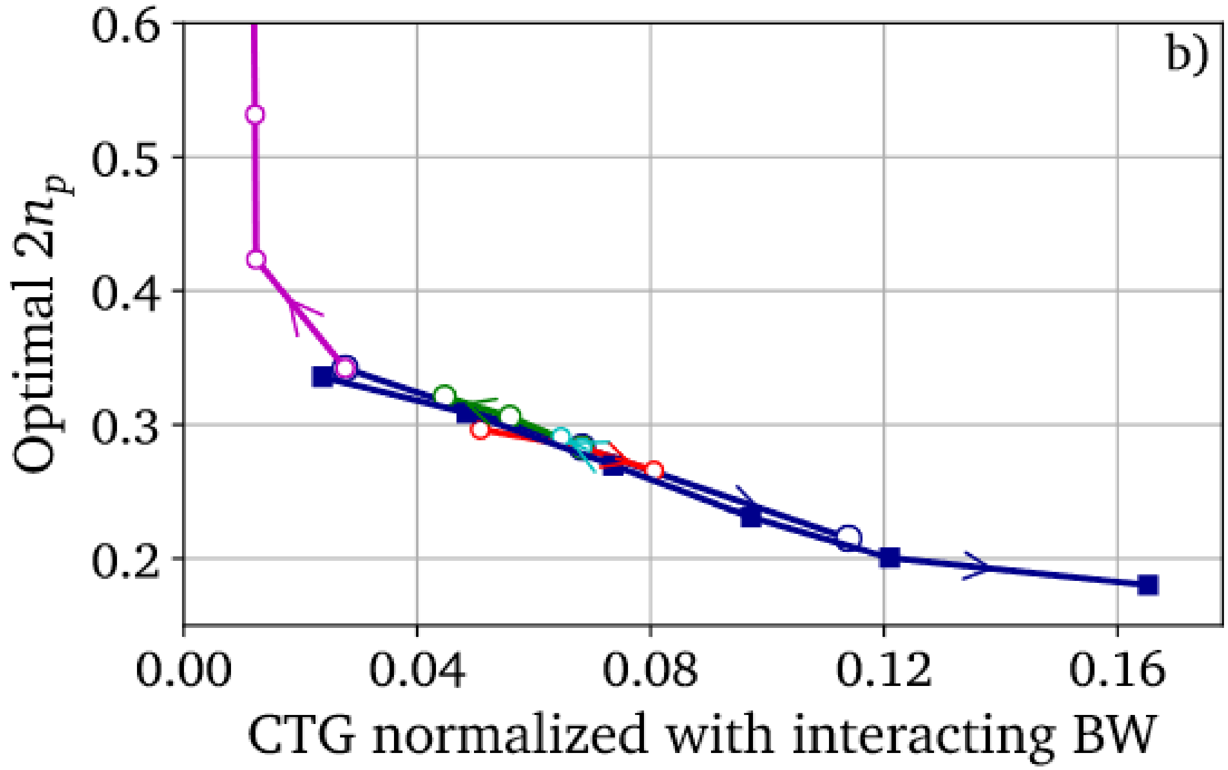


Weber, Yee, Haule, Kotliar, EPL 100, 2012



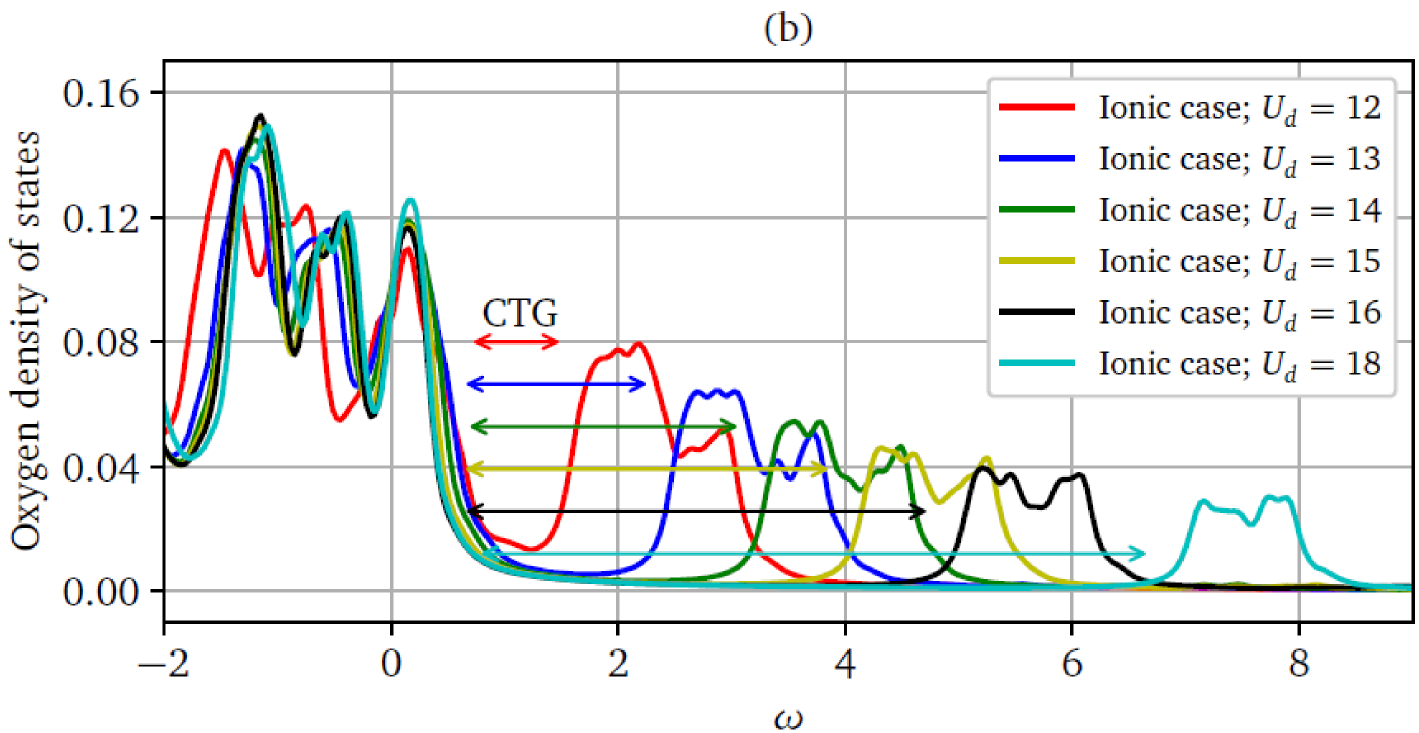
Kowalski, Dash, Sémon, Sénéchal, A-M.T.
PNAS **118** (40) e2106476118 (2021)

Charge-transfer gap, oxygen hole content



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

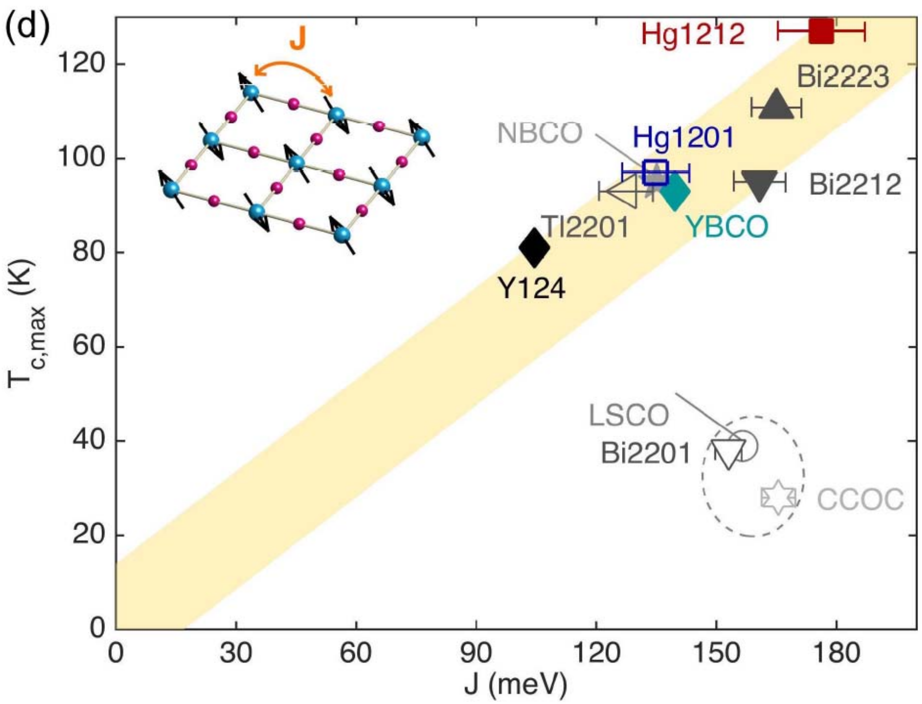
Charge transfer gap and oxygen hole content : Oxygen as a witness

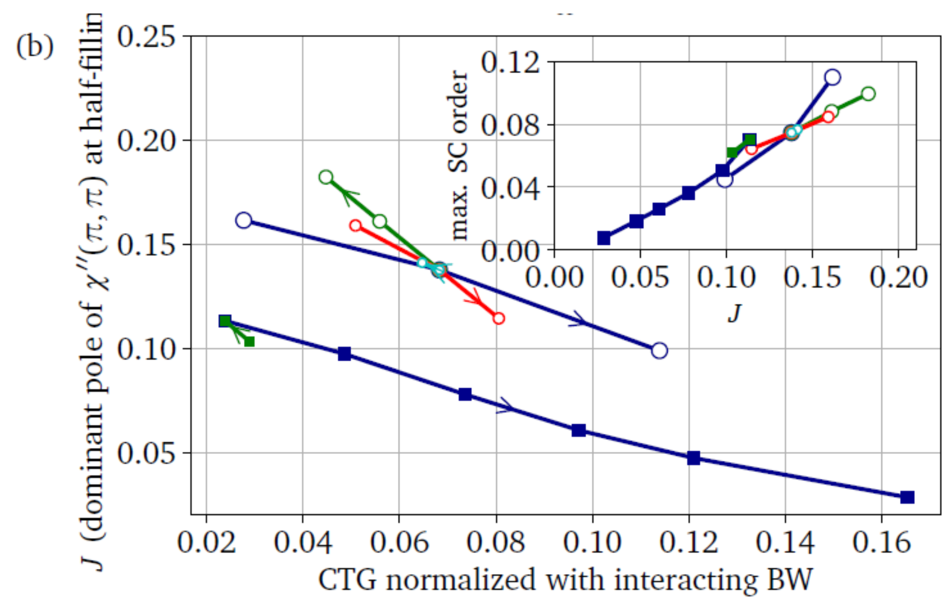


© Sidhartha Dash

Copper pairing mechanism : superexchange

#3 Optimizing T_c with superexchange





Lichen Wang, *et al.* arXiv 2011.05029

$J = 4t^2/U$

D. Sénéchal

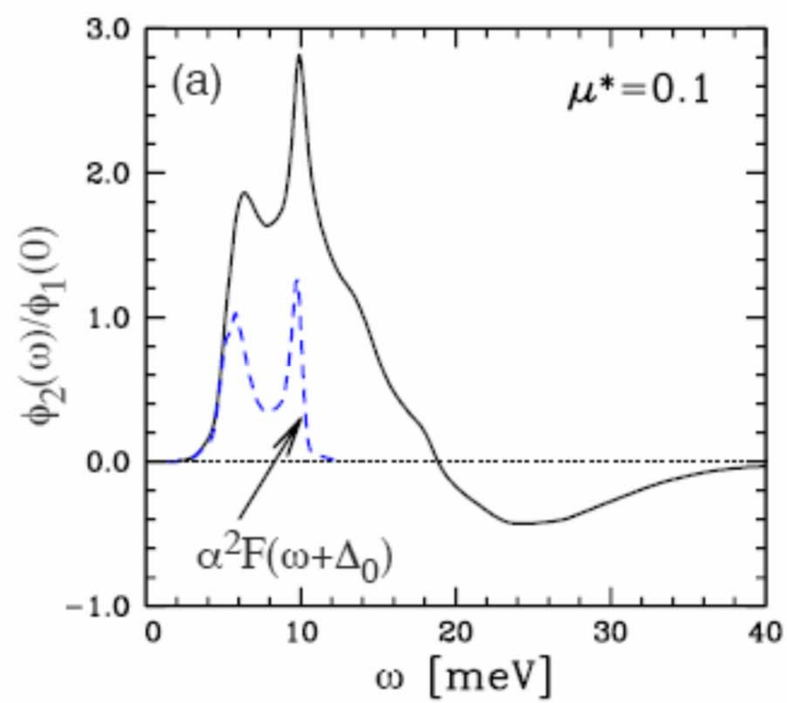
Bumsoo Kyung

The glue

Kyung, Sénéchal, Tremblay, Phys. Rev. B **80,** 205109 (2009)
Sénéchal, Day, Bouliane, AMST, Phys. Rev. B **87**, 075123 (2013)
A. Reymbaut *et al*. PRB **94** 155146 (2016)

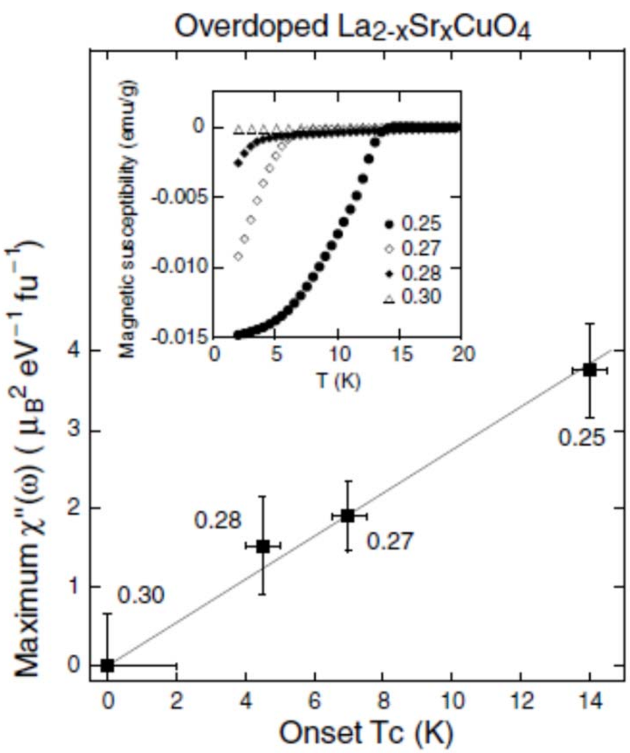
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

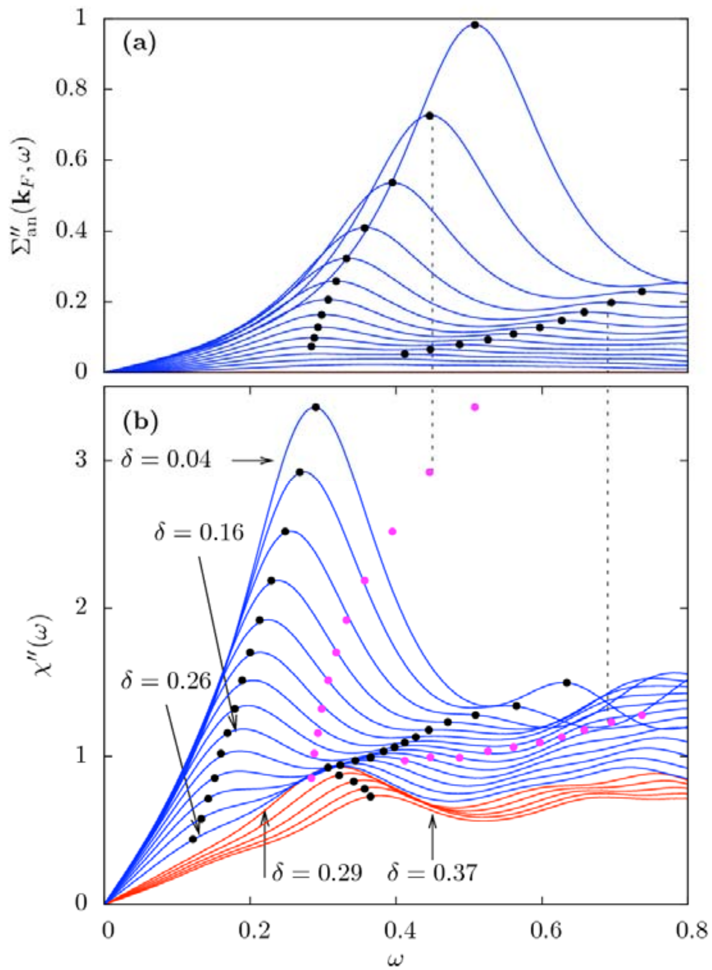


The glue CDMFT 2x2, T=0

Kyung, Sénéchal, Tremblay, Phys. Rev. B **80,** 205109 (2009)

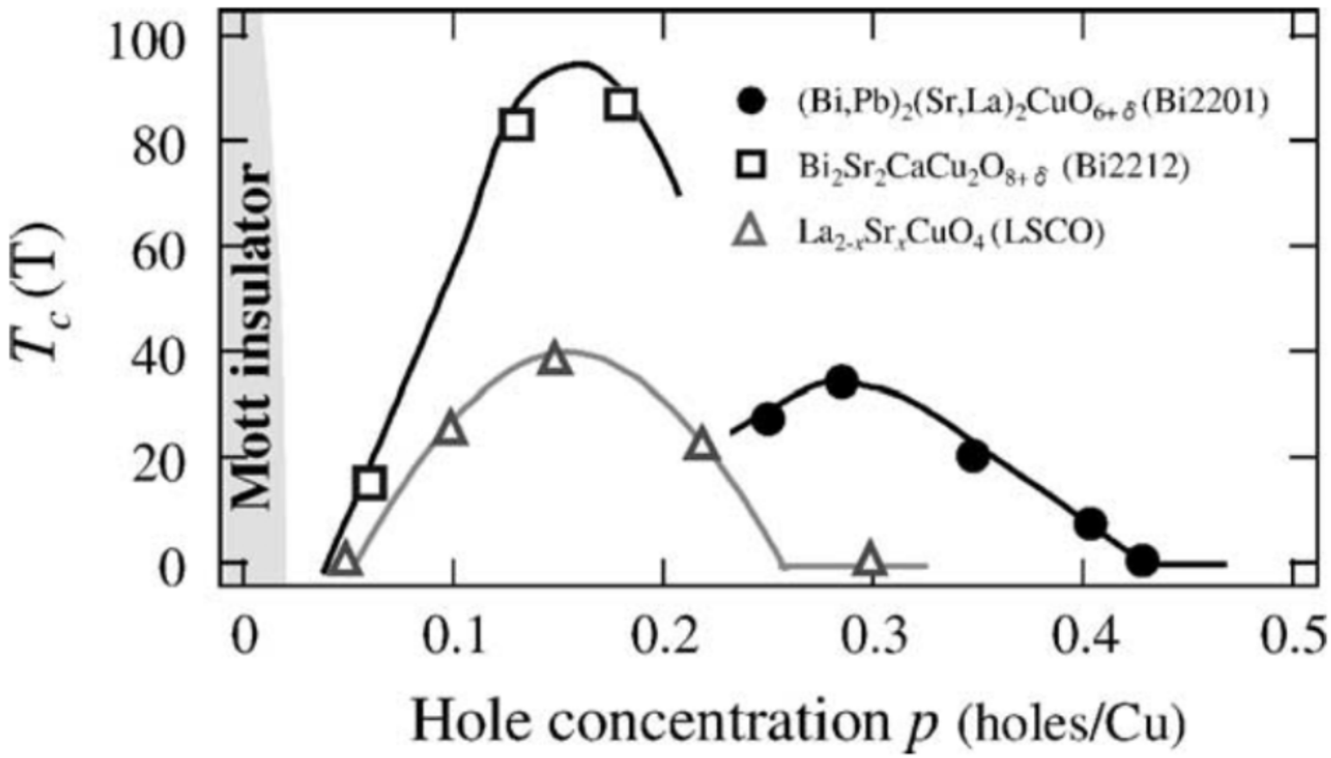


Wakimoto … Birgeneau PRL (2004)



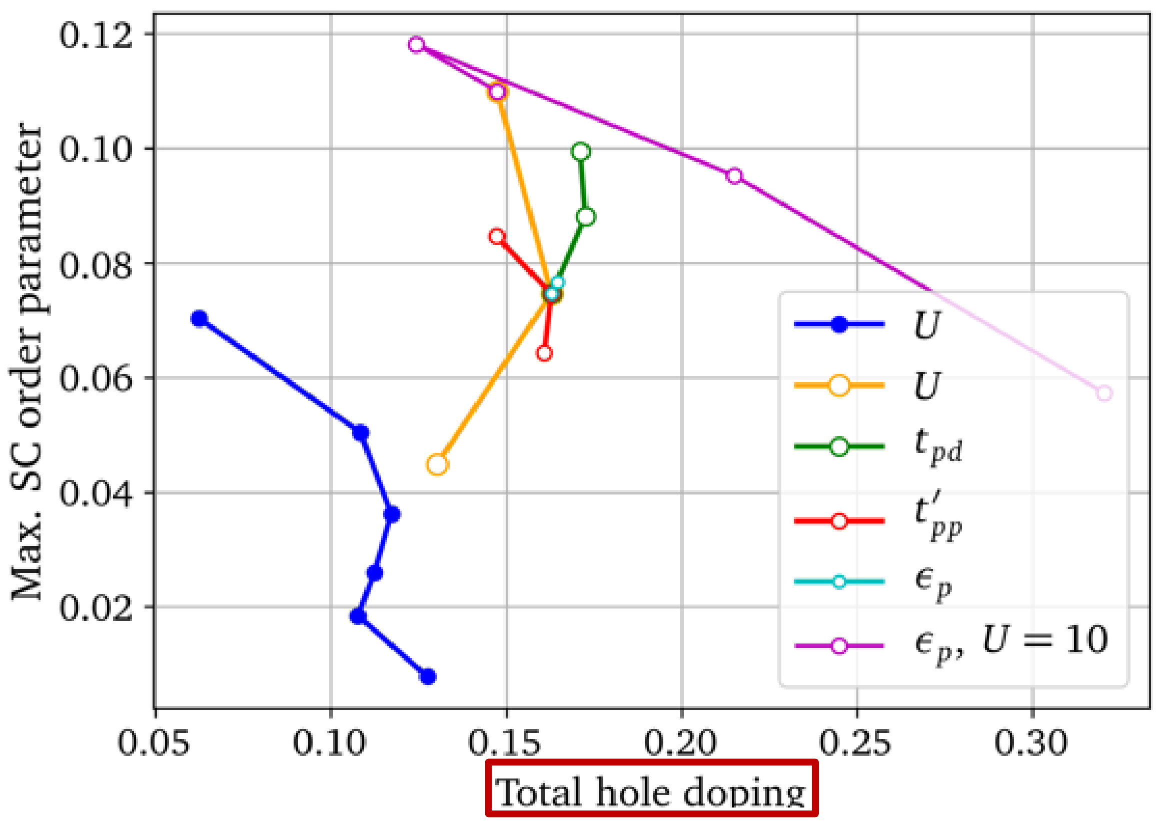
Bonus

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)

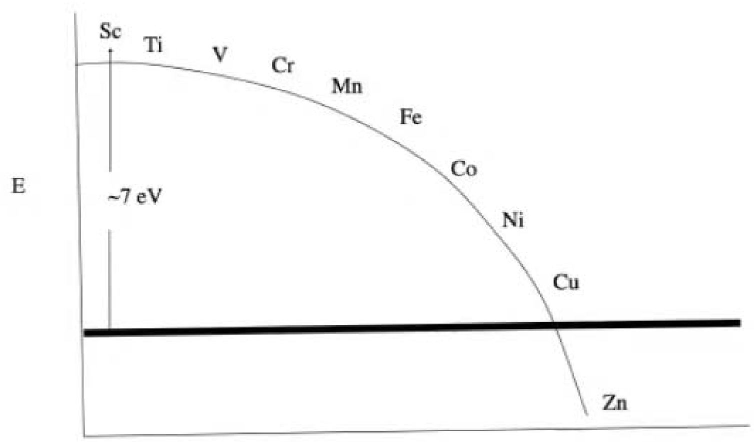
Bonus: total hole doping does not explain max order parameter for the two models



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

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Optimizing Tc

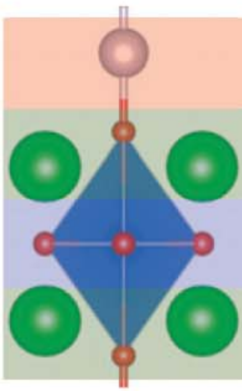
- Spin ½
- One band
- Two-dimensions
- Strong covalency between chalchogen and transition metal.
  - Chalcogen screens U
- Charge-transfer gap just opening (intermediate interactions).
- Large *J* at half-filling
- … and more

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)

Optimizing T_c



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BaO	neutral	inert	protects CuO_2 from disorder	tunes in-plane t, t', U
CuO_2	-2 charge/u.c.	accepts	roughly sets lattice const.	superconducts
BaO	(same as other CaS layer)			

$$Hg(CaS)_2CuO_2$$

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

Merci
Thank you

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