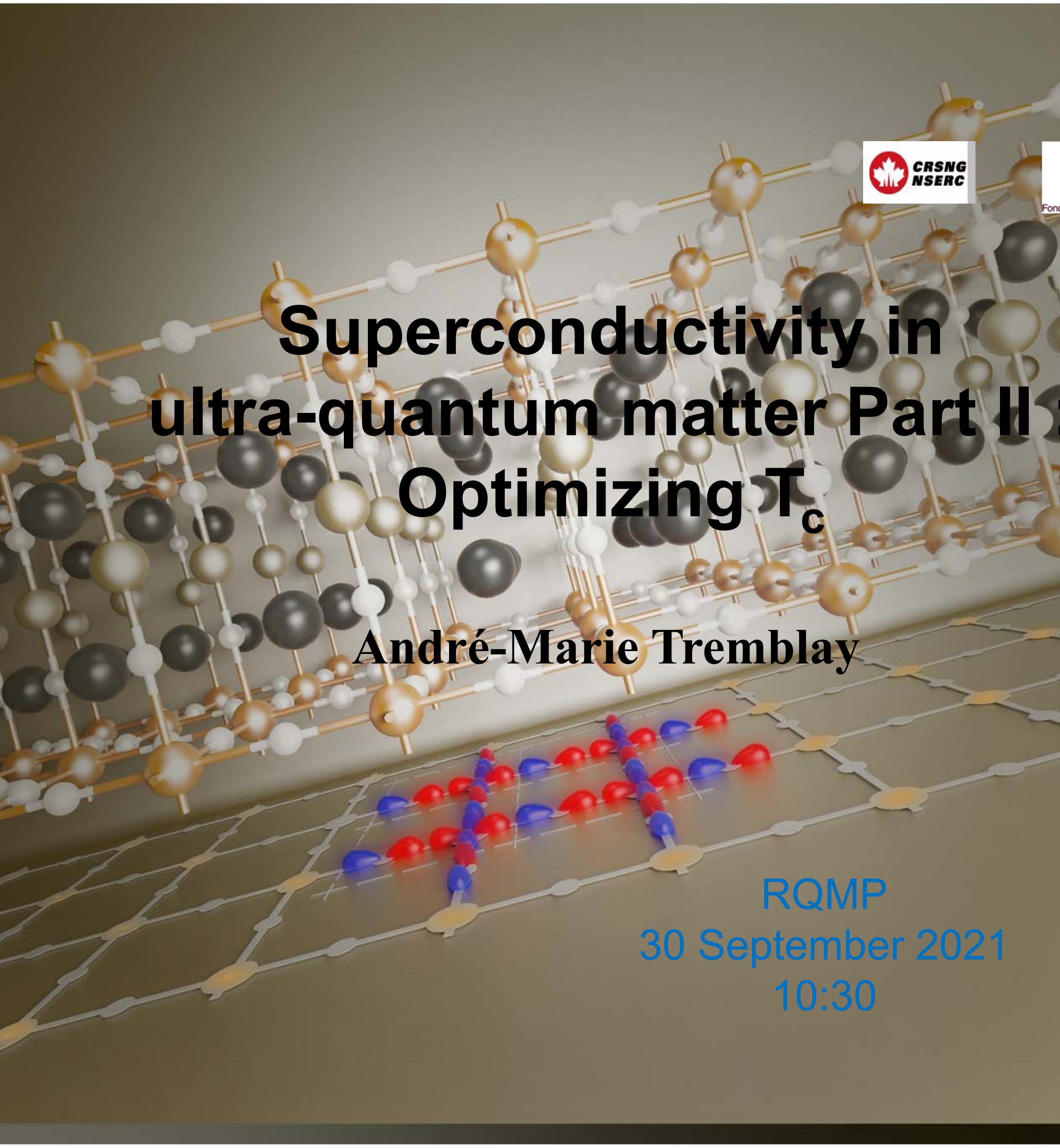
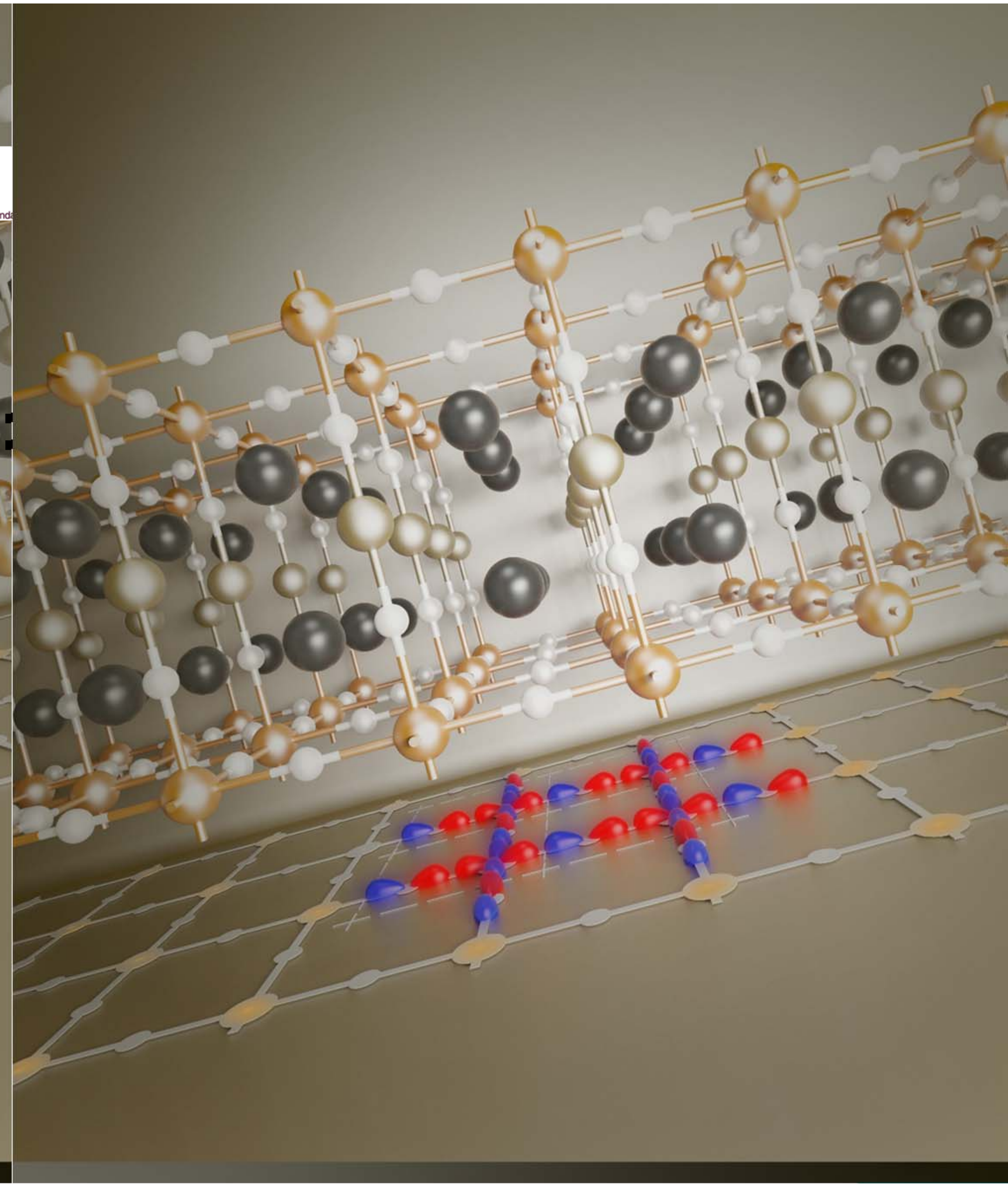


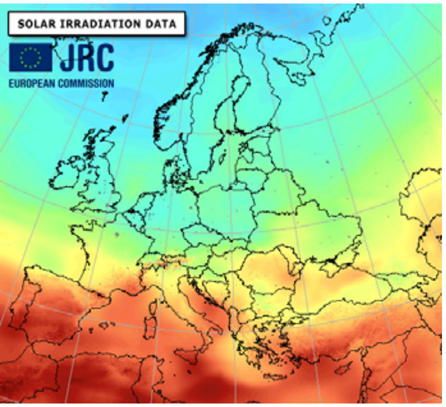
Superconductivity in ultra-quantum matter Part II : Optimizing T_c

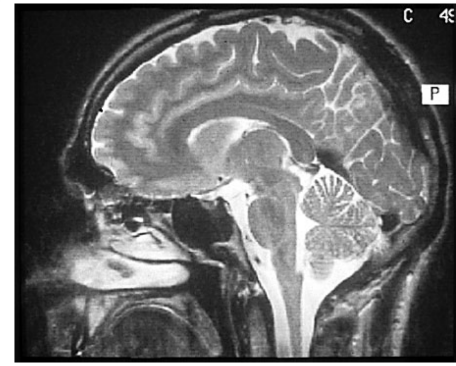
André-Marie Tremblay

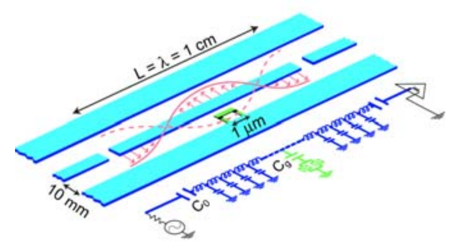
RQMP
30 September 2021
10:30



Applications



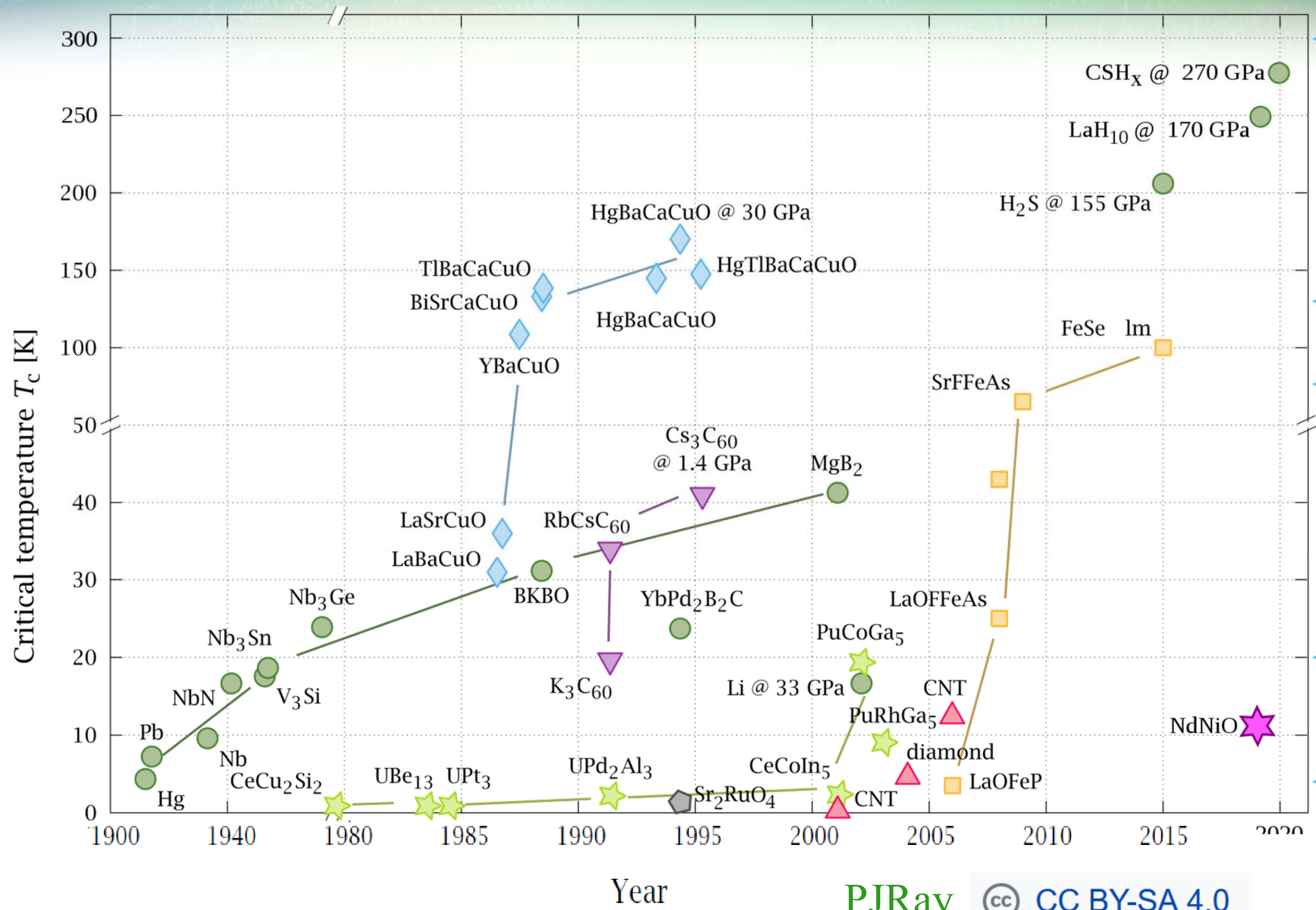




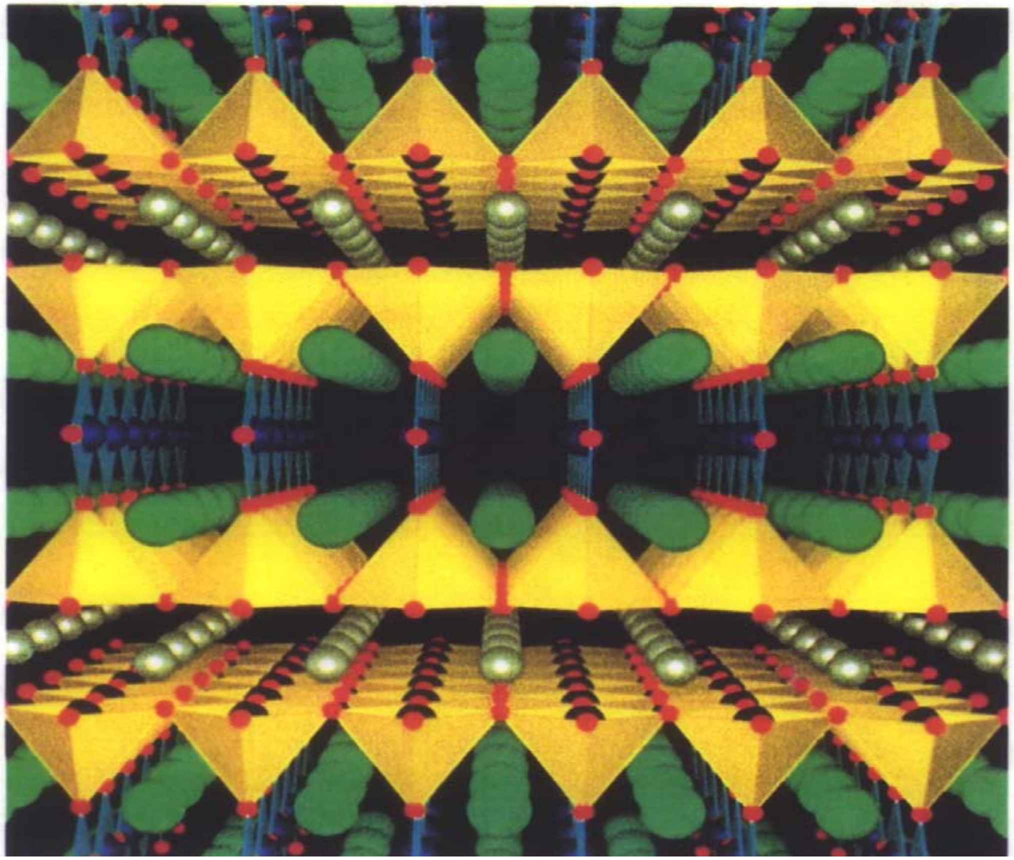
Alexandre Blais, et al. Phys. Rev. A **69**, 062320 (2004)

Photo IBM

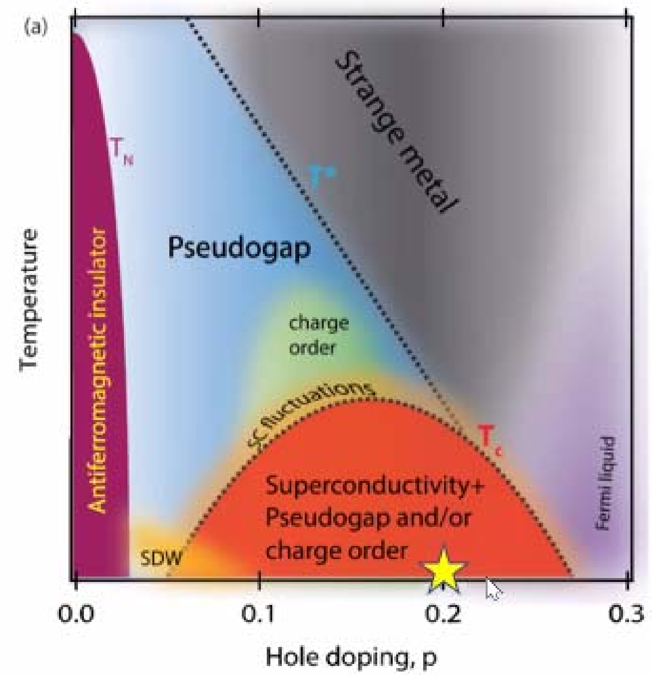
Can we have superconductivity at room temperature?


Critical temperature T_c [K]
Year
CSH$_x$ @ 270 GPa
LaH$_{10}$ @ 170 GPa
H$_2$S @ 155 GPa
HgBaCaCuO @ 30 GPa
HgTlBaCaCuO
TlBaCaCuO
BiSrCaCuO
HgBaCaCuO
YBaCuO
FeSe lm
SrFFeAs
Cs$_3$C$_{60}$
@ 1.4 GPa
MgB$_2$
LaSrCuO
RbCsC$_{60}$
LaBaCuO
BKBO
YbPd$_2$B$_2$C
LaOFFeAs
Nb$_3$Ge
Nb$_3$Sn
PuCoGa$_5$
NbN
V$_3$Si
K$_3$C$_{60}$
Li @ 33 GPa
CNT
PuRhGa$_5$
NdNiO
Pb
Nb
diamond
CeCu$_2$Si$_2$
UBe$_{13}$
UPt$_3$
UPd$_2$Al$_3$
CeCoIn$_5$
LaOFeP
Hg
Sr$_2$RuO$_4$
CNT
0
10
20
30
40
50
100
150
200
250
300
1900
1940
1980
1985
1990
1995
2000
2005
2010
2015
2020

Cuprates : Atomic structure



- Who ordered this?

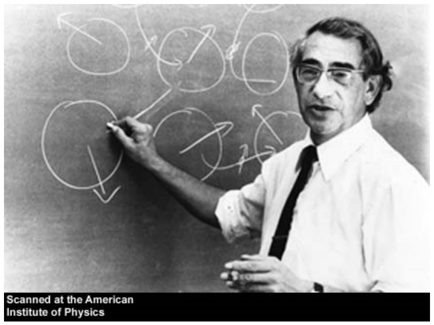


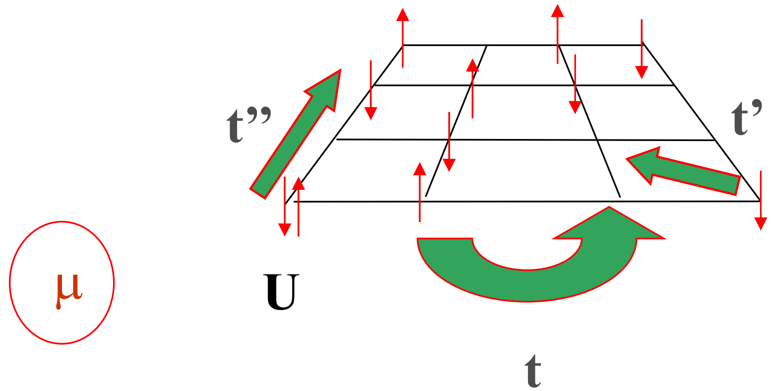
Vishik, Rep. Prog. Phys. (2018)

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

A highly quantum mechanical problem

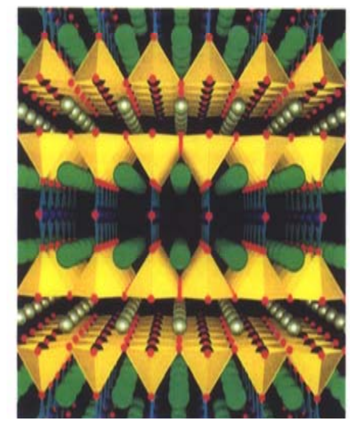
Hubbard model



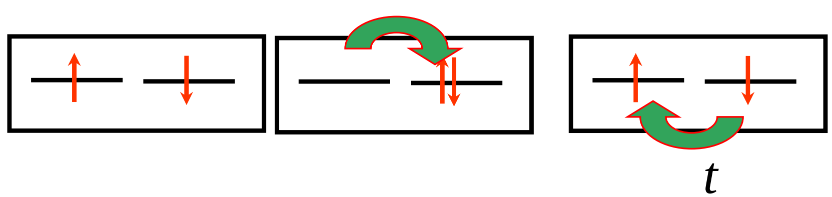


1931-1980

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



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
  - Explaining 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

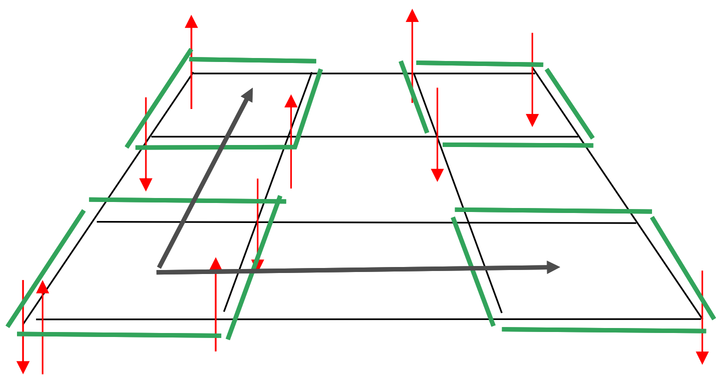
Method

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

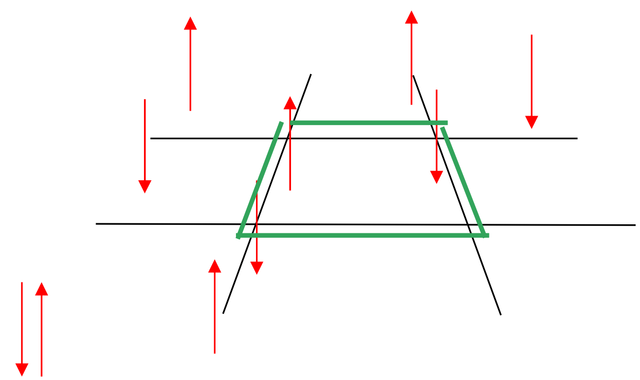
Localized and delocalized pictures C-DMFT

Delocalized



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

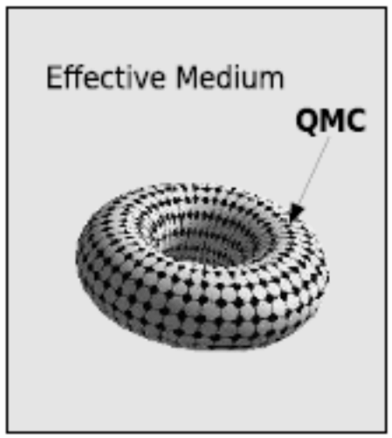
Localized

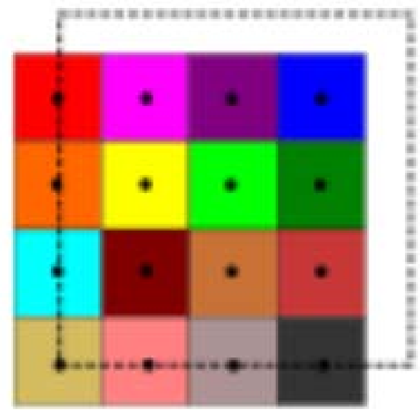


$$G_{ij} = \int \frac{d^d\tilde{k}}{(2\pi)^d} \left(\frac{1}{(i\omega_n+\mu)I - \varepsilon(\tilde{k}) - \Sigma} \right)_{ij}$$

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

Dynamical cluster approximation (DCA)

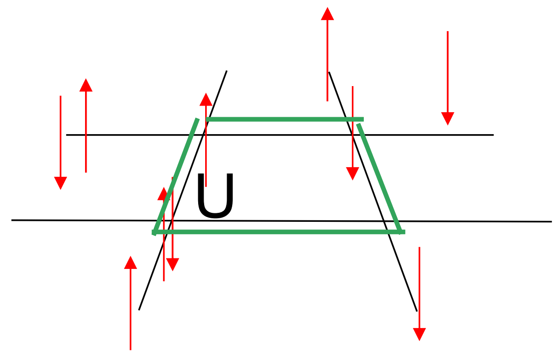




Hettler …Jarrell…Krishnamurty PRB **58** (1998)

Impurity solvers

Impurity solver (Exact diagonalisation)



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

QCM David Sénéchal

Impurity solver : continuous-time quantum Monte Carlo

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

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, Wu (Paris)
  - Lichtenstein, Potthoff, (Hamburg) Aichhorn (Graz), Liebsch (Jülich) de Medici (Grenoble) Capone (Italy)
- USA:
  - Gull (Michigan) Millis (Columbia)
  - Kotliar, Haule (Rutgers)
  - Jarrell (Louisiana)
  - Maier, Okamoto (Oakridge)
- Japan
  - Imada (Tokyo) Sakai, Tsunetsugu, Motome

Critique

+ and -

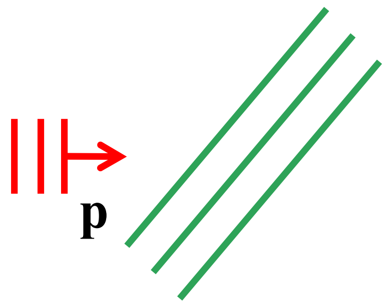
- Long range order:
  - No mean-field factorization on the cluster
  - Symmetry breaking allowed in the bath
- Included exactly:
  - Short-range dynamical and spatial correlations

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

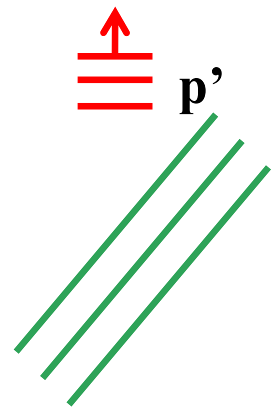
d-wave superconductivity One band model

Superconductivity

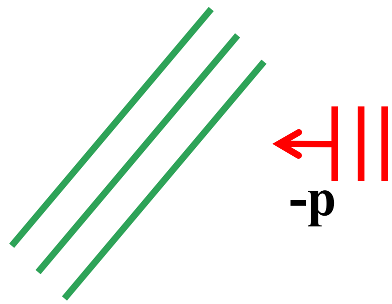
Attraction mechanism in the metallic state



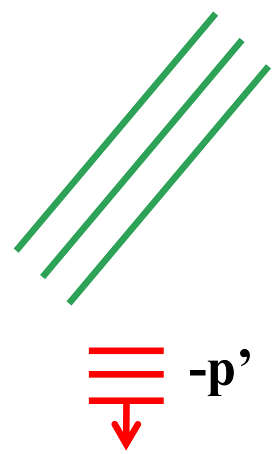
Attraction mechanism in the metallic state



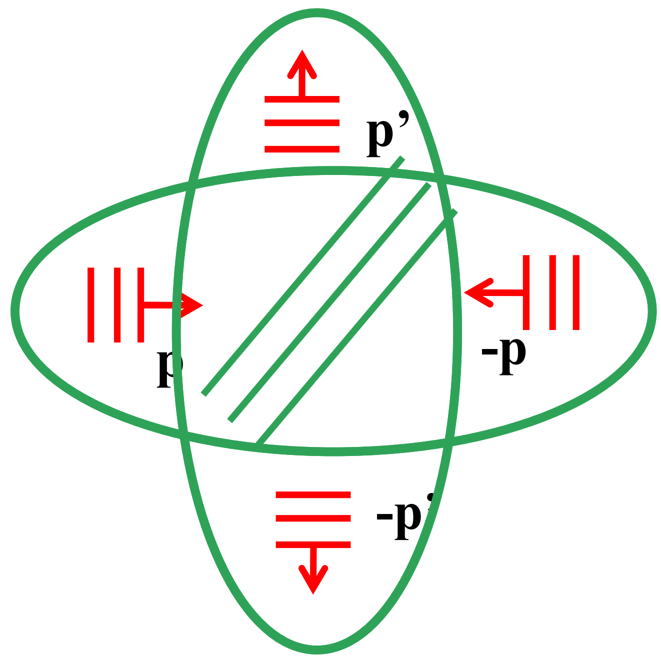
Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



Attraction mechanism in the metallic state



#1 Cooper pair, #2 Phase coherence

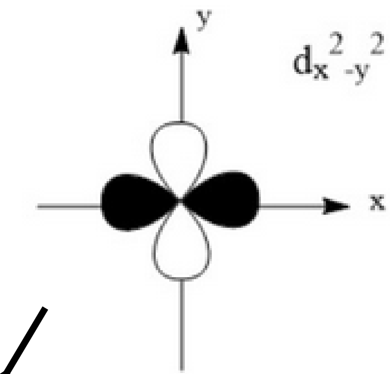
$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow}$$

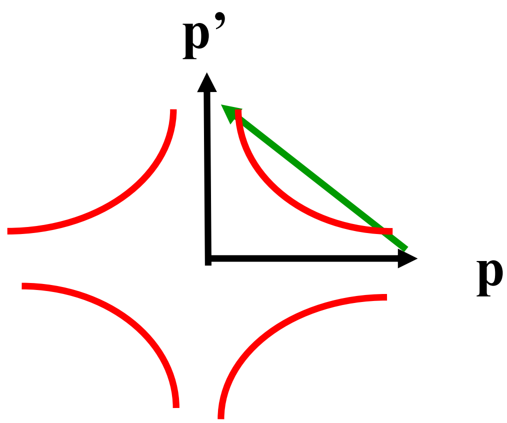
$$E_P = \sum_{\mathbf{p},\mathbf{p}'} U_{\mathbf{p}-\mathbf{p}'} \left\langle \psi^*_{\mathbf{p}'\uparrow,-\mathbf{p}'\downarrow} \right\rangle \left\langle \psi_{\mathbf{p}\uparrow,-\mathbf{p}\downarrow} \quad \right\rangle$$

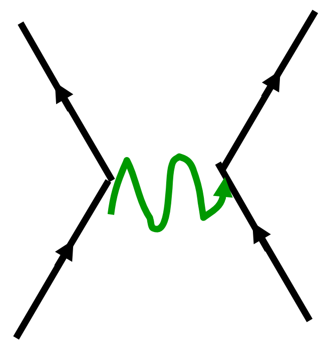
$$|\mathrm{BCS}(\theta)\rangle = \ldots + e^{iN\theta}|N\rangle + e^{i(N+2)\theta}|N+2\rangle + \ldots.$$

Cartoon « BCS » weak-coupling picture

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





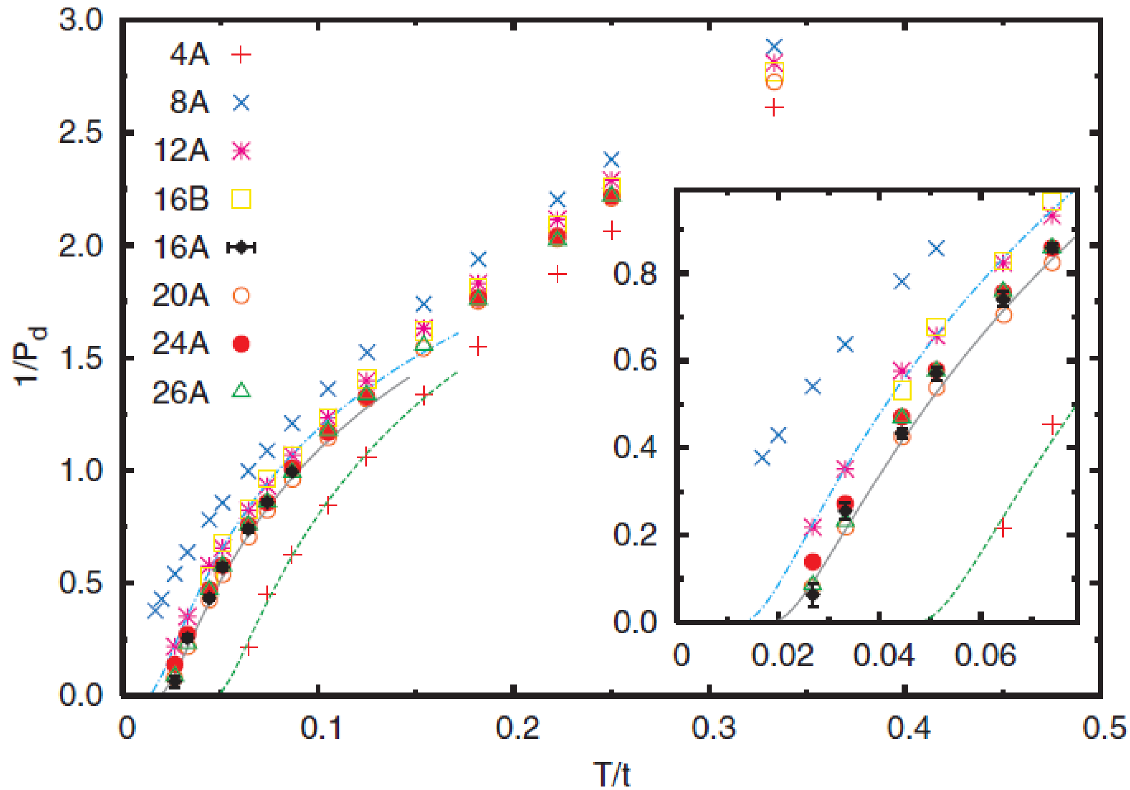


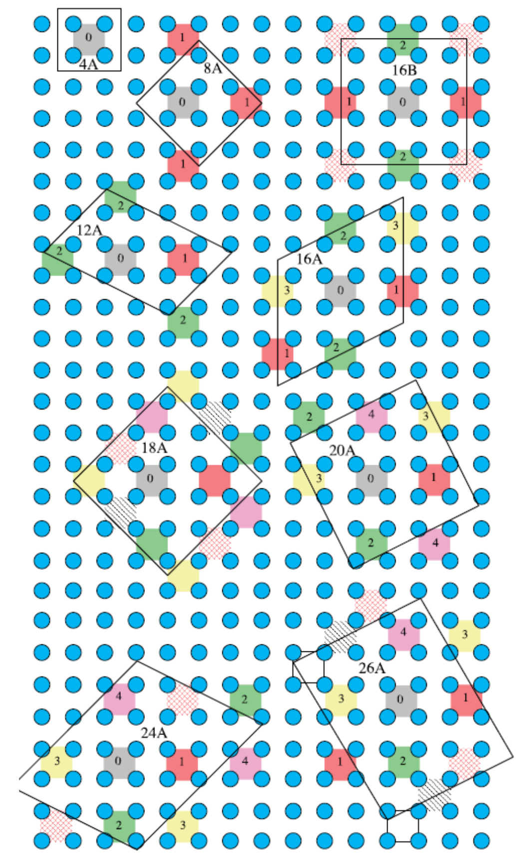
Béal–Monod, Bourbonnais, Emery
P.R. B. **34**, 7716 (1986).
D. J. Scalapino, E. Loh, Jr., and J. E. Hirsch
P.R. B **34**, 8190-8192 (1986).
Kohn, Luttinger, P.R.L. **15**, 524 (1965).

Exchange of spin waves?
Kohn-Luttinger
T_c with pressure

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

Exchange of spin waves, *U = 4t doping 10%*



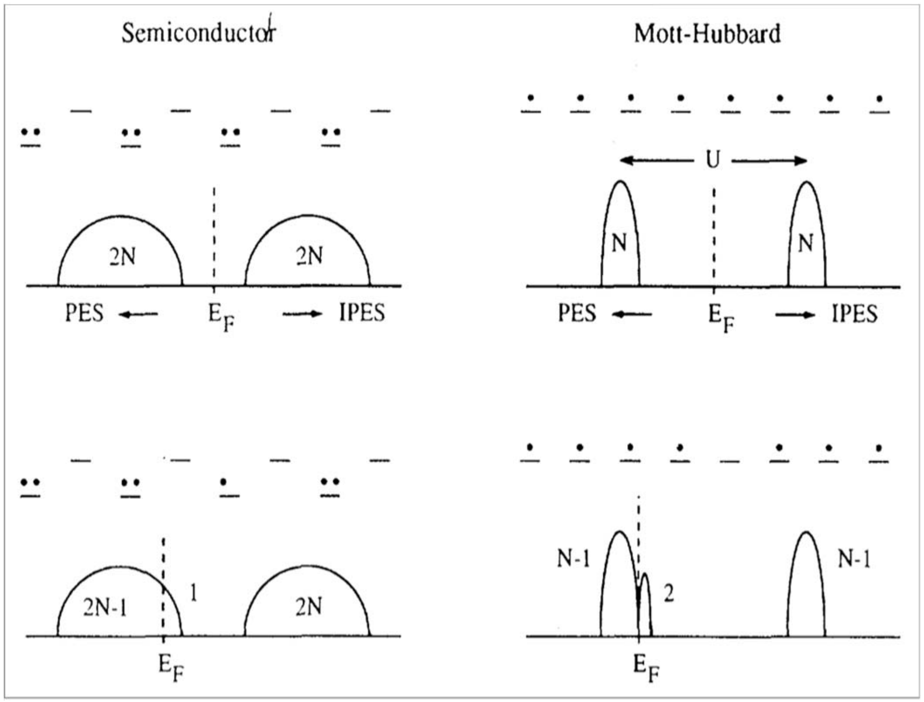


Maier, Jarrell, Schulthess, Kent, White PRL **95,** 237001 (2005)

The strong-correlation limit : Superexchange

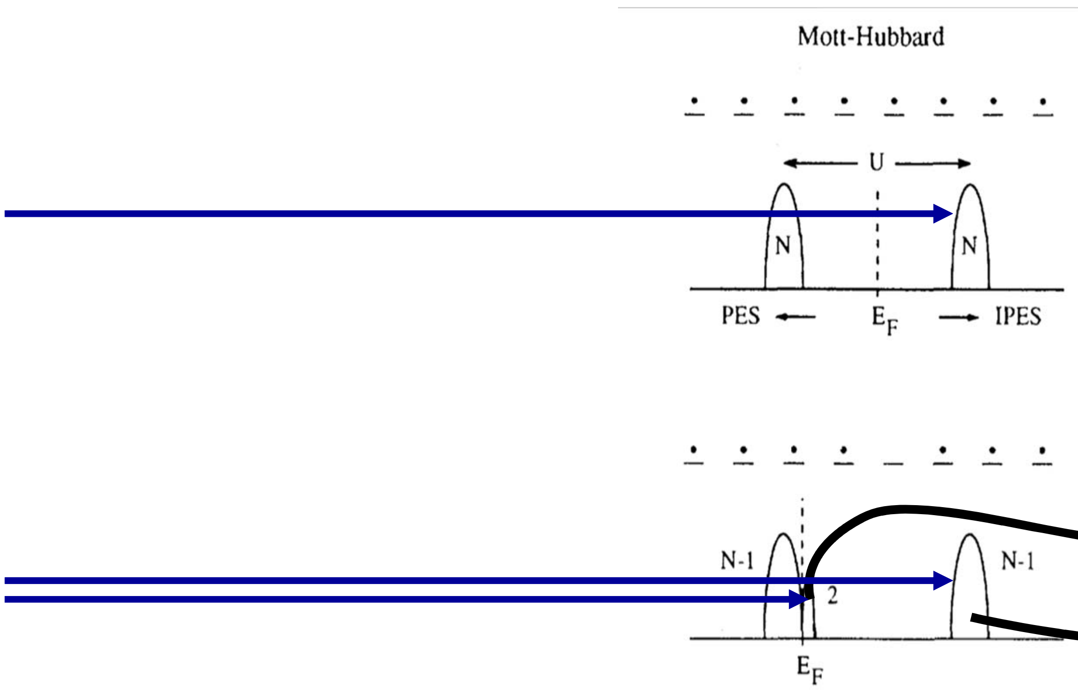
Mott Insulator

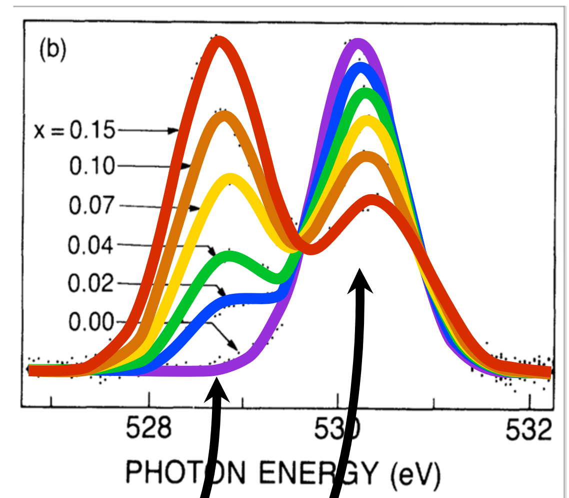
Meinders *et al.* PRB **48**, 3916 (1993)



Mott Insulator : X-Ray absorption

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





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

A cartoon strong correlation picture

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

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

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

Pitaevskii Brückner:

Pair state orthogonal to repulsive core of Coulomb interaction

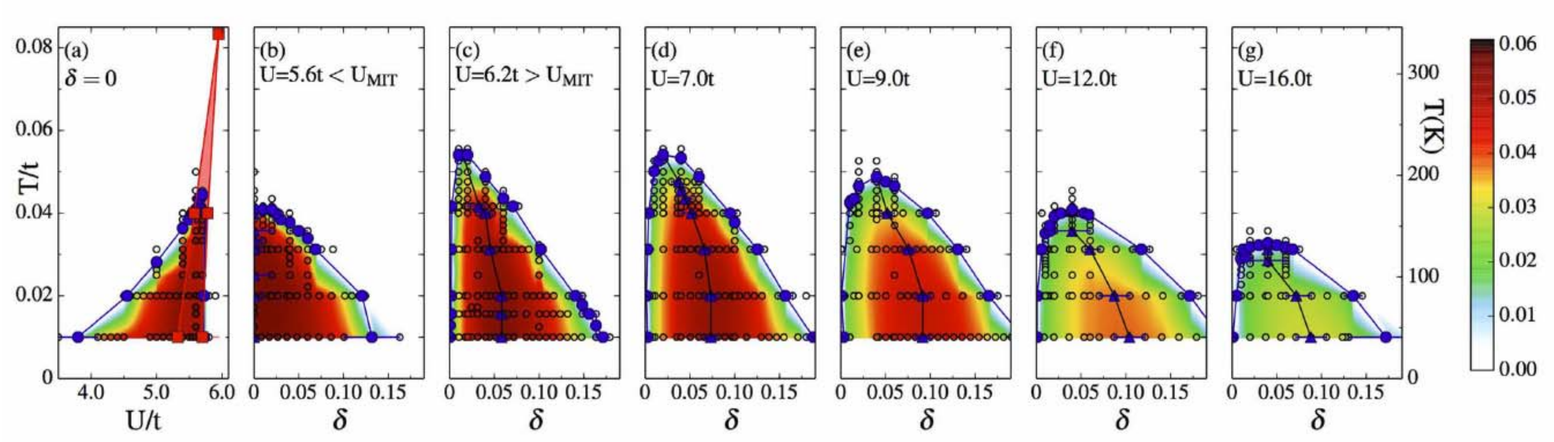
P.W. Anderson Science 317, 1705 (2007)

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

More sophisticated Slave Boson: Kotliar Liu PRB 1988

T_c controlled by *J*, CDMFT *2x2*

J = 4t² /U



Fratino et al.
Sci. Rep. **6**, 22715

Some experiments that suggest $T_c < T_{pair} < T^*$

T. Kondo *et al*. PRL **111** (2013)

Kondo, Takeshi, et al. Kaminski Nature Physics 2011, **7**, 21-25

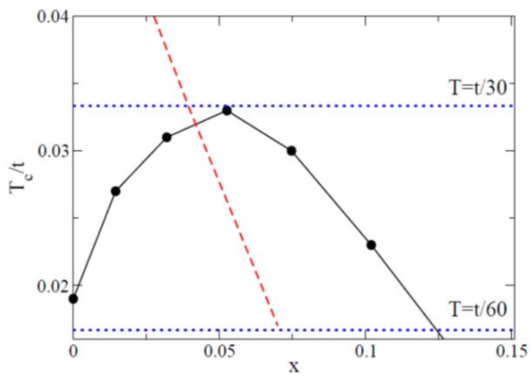
A. Pushp, Parker, … A. Yazdani, Science **364**, 1689 (2009)

Lee …Tajima (Osaka) https://arxiv.org/pdf/1612.08830

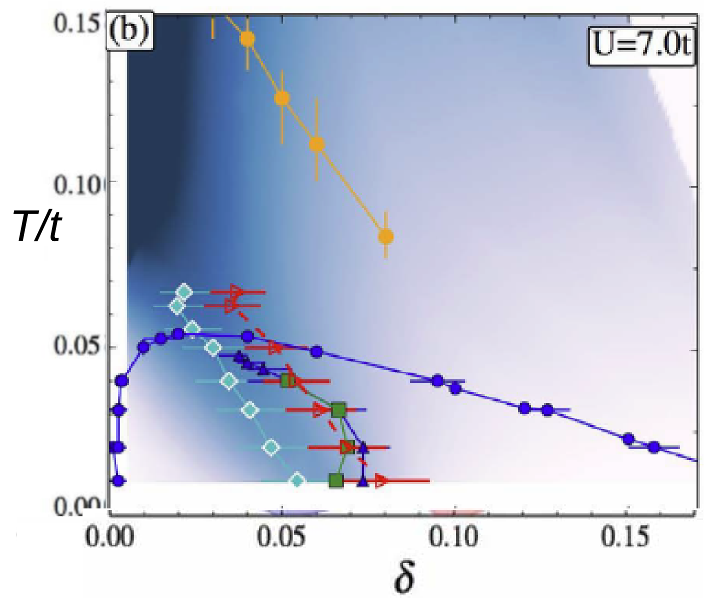
Patrick M. Rourke, et al. Hussey Nature Physics **7,** 455–458 (2011)

Lee et al. J. Phys. Soc. Jpn. 86, 023701 (2017)

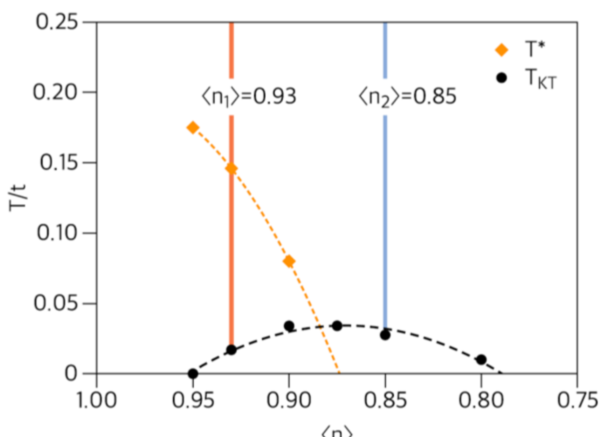
Phase diagram



E. Gull and A. J. Millis
Phys. Rev. B 88, 075127

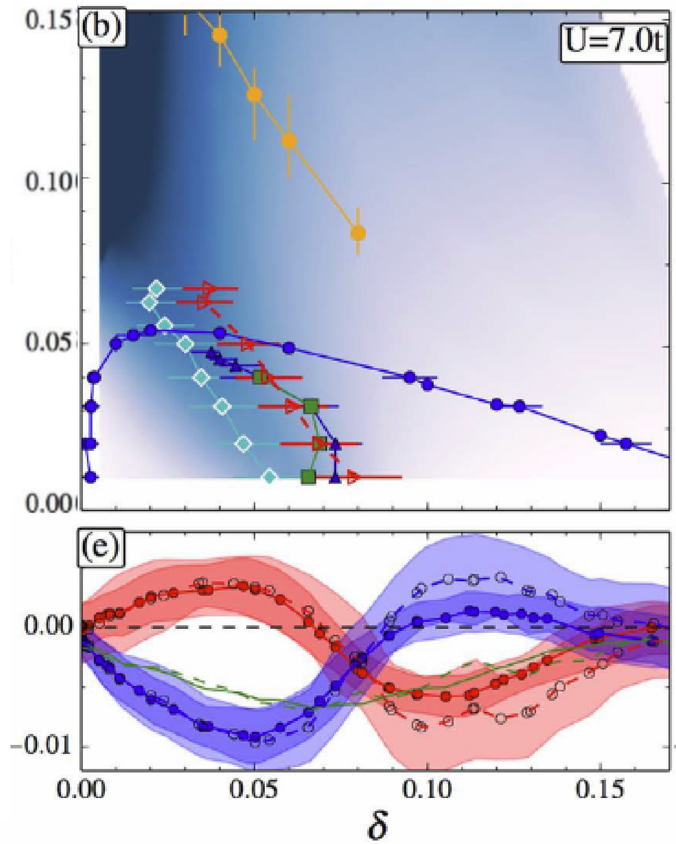


Fratino et al.
Sci. Rep. **6**, 22715



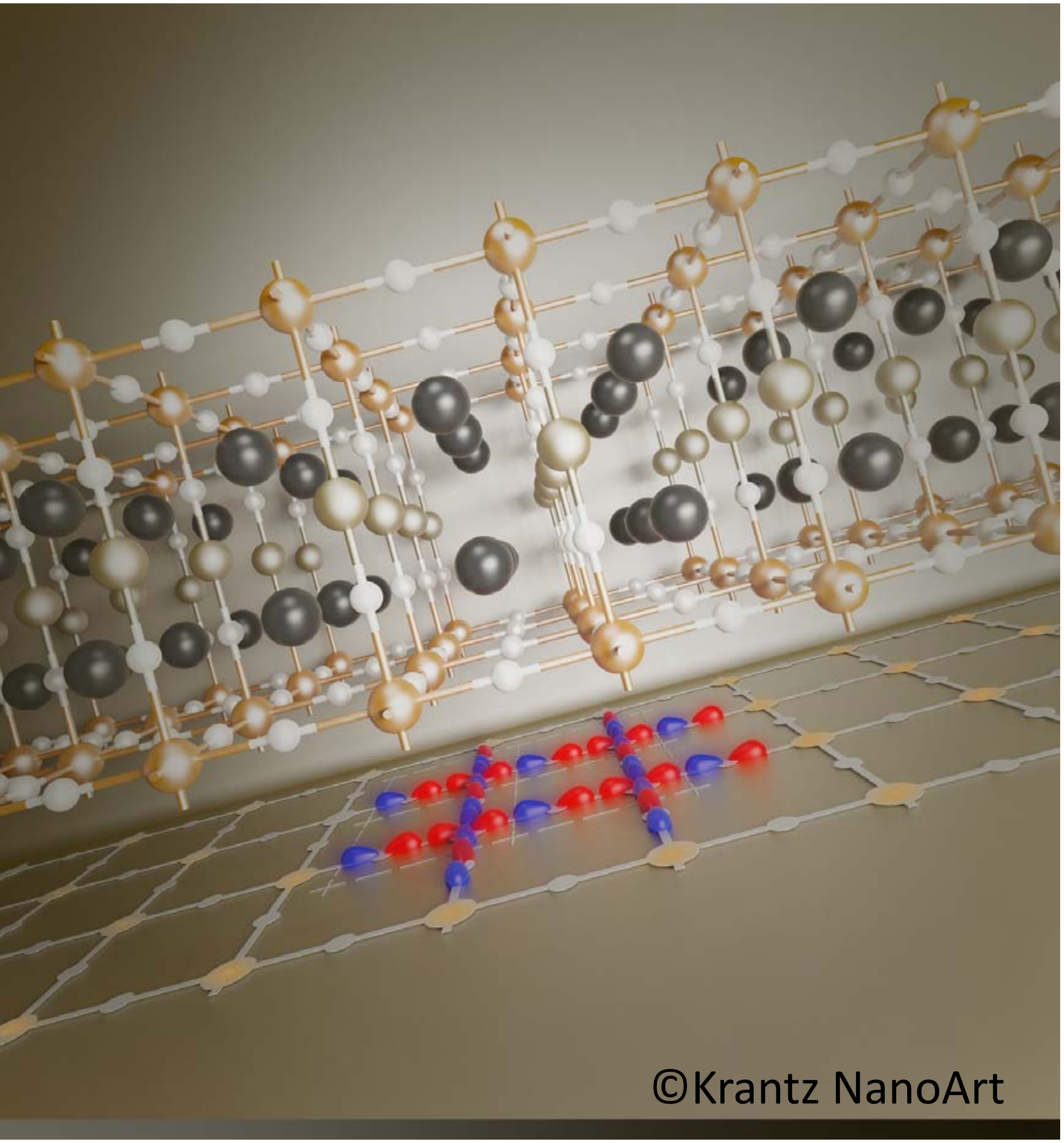
T.A. Maier, D.J. Scalapino, npj Quantum Materials (2019)

Condensation energy



Fratino et al.
Sci. Rep. **6**, 22715

Theory, see also Jarrel PRL (2004), Gull Millis PRB (2014)
Experiments: Bontemps, Santander-Syro Van der Marel …



USHERBROOKE.CA/IQ

Three-band (Emery VSA) Hubbard model


Sidhartha Dash


Nicolas Kowalski


Patrick Sémon


David Sénéchal

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

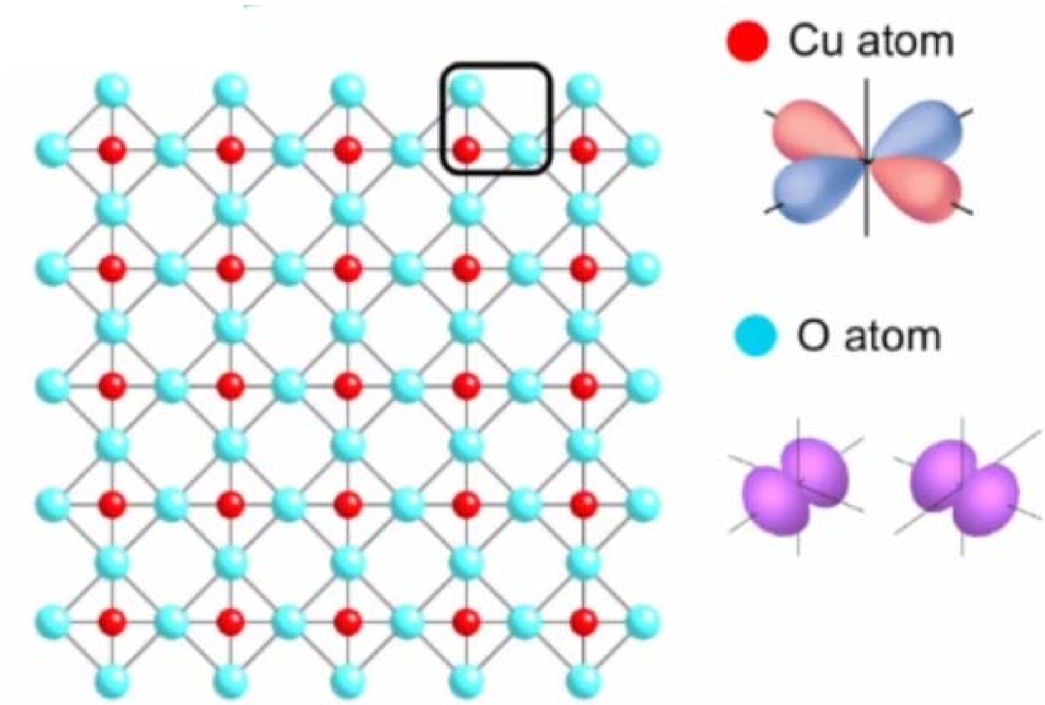
C. M. Varma, S. Schmitt-Rink, and E. Abrahams, Solid State Communications **62**, 681–685 (1987), ISSN 0038-1098,

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

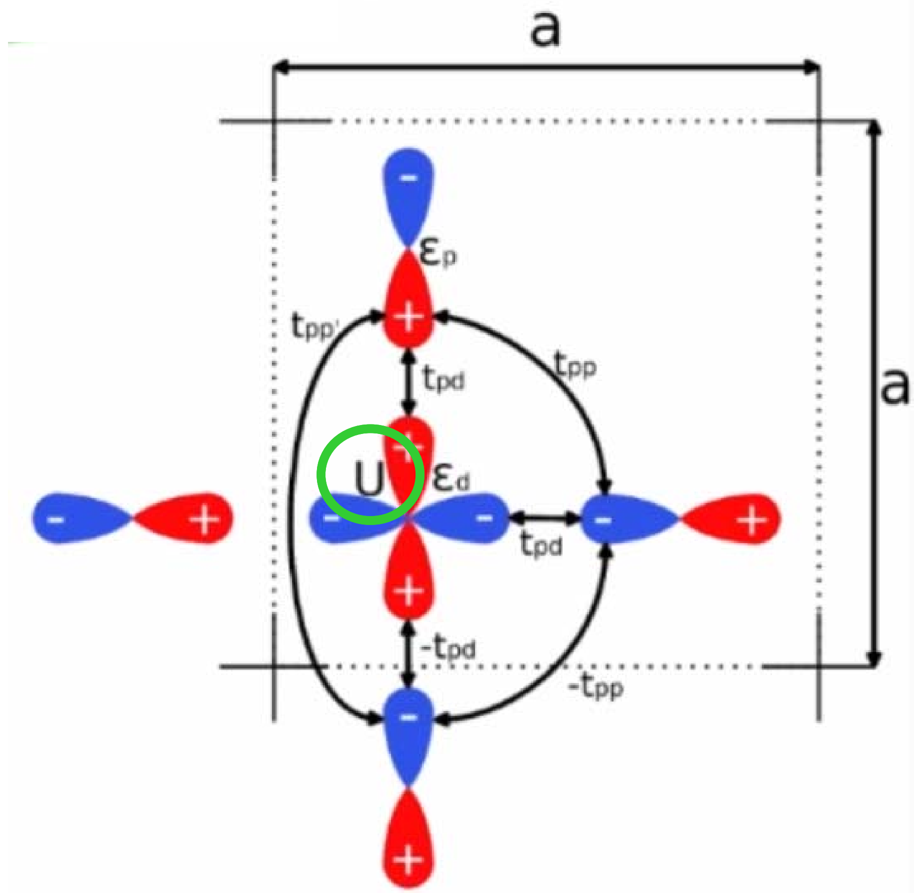
UNIVERSITÉ DE SHERBROOKE

USHERBROOKE.CA/IQ

Copper and oxygen planes

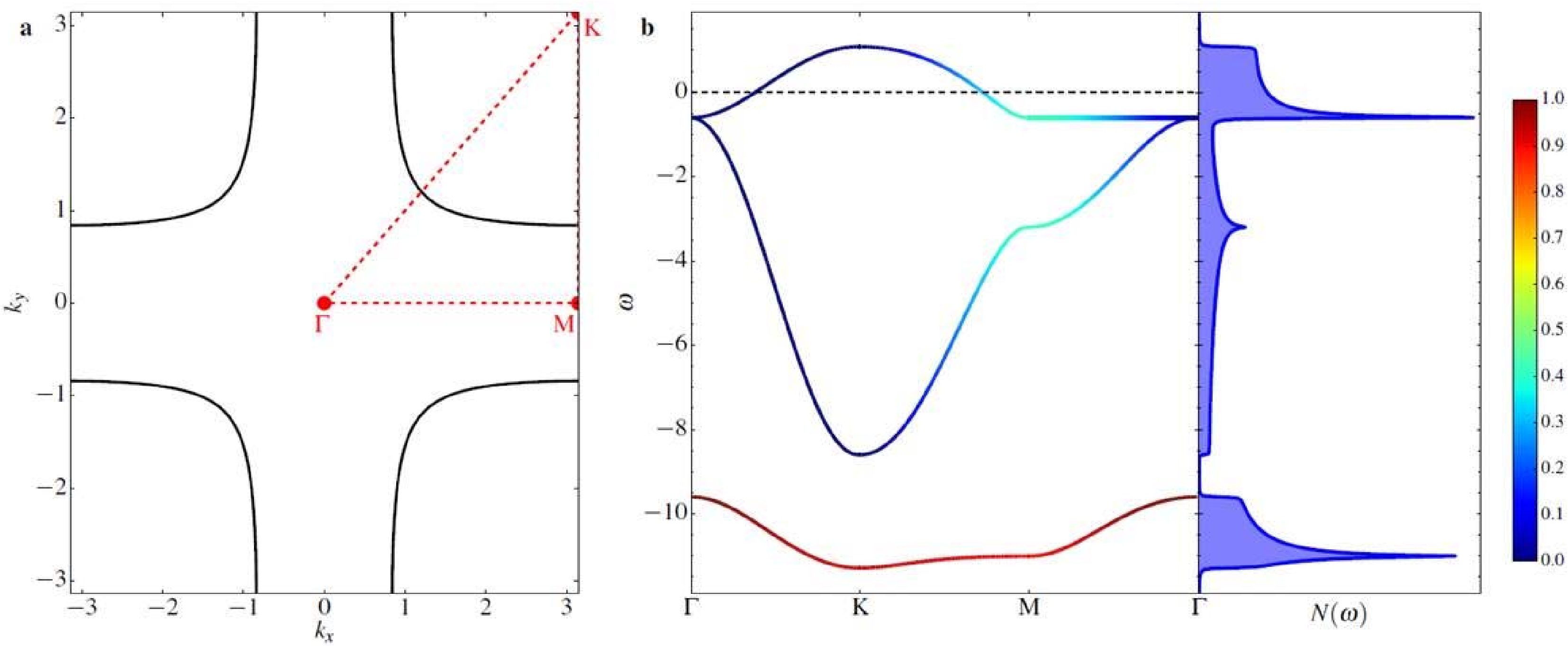


© Nicolas Kowalski



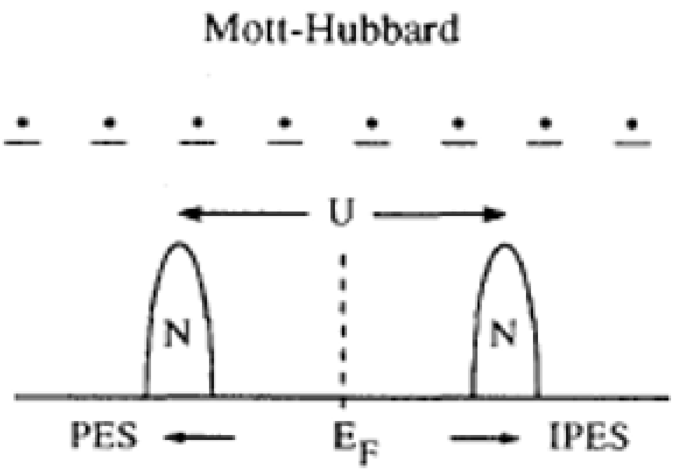
© Nicolas Kowalski

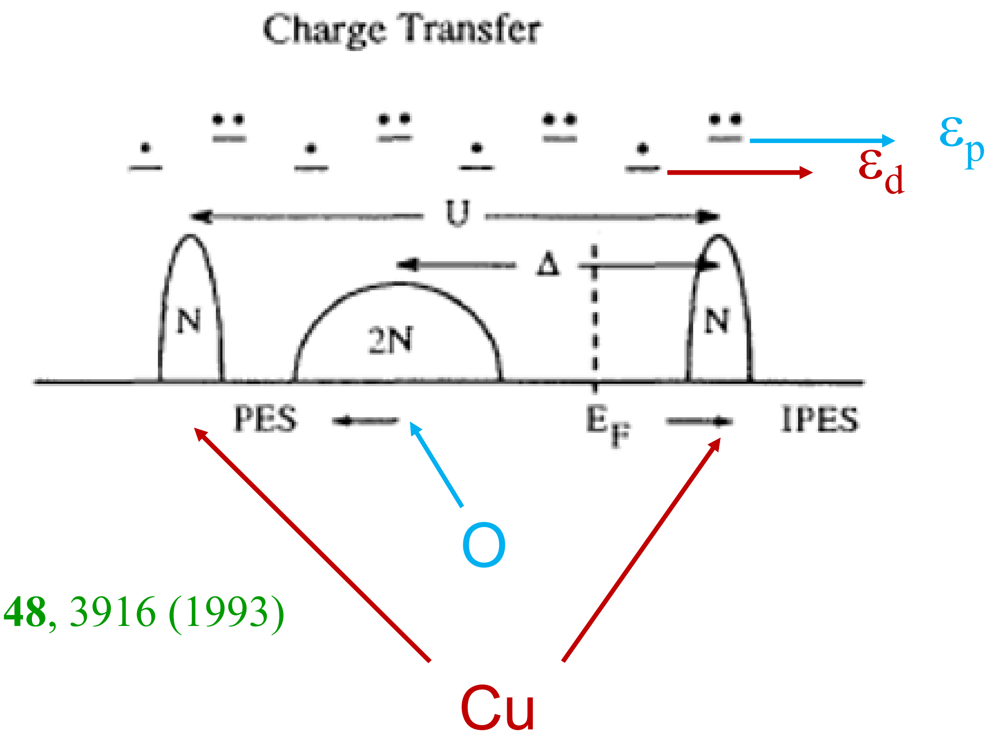
Bands : Copper-Oxygen hybridization



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

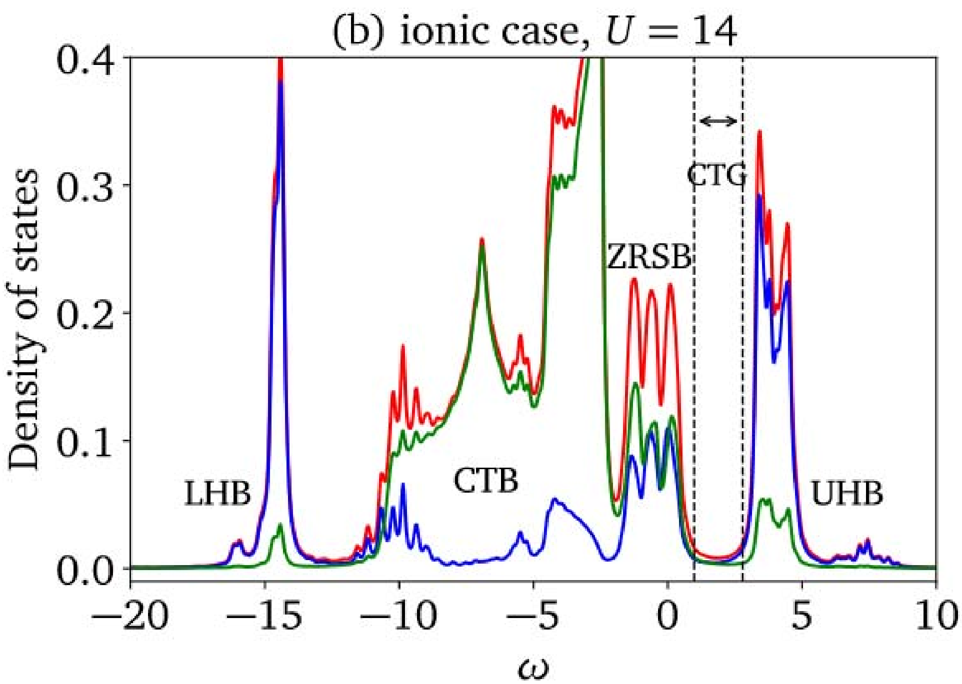
Interactions : Charge-transfer insulator

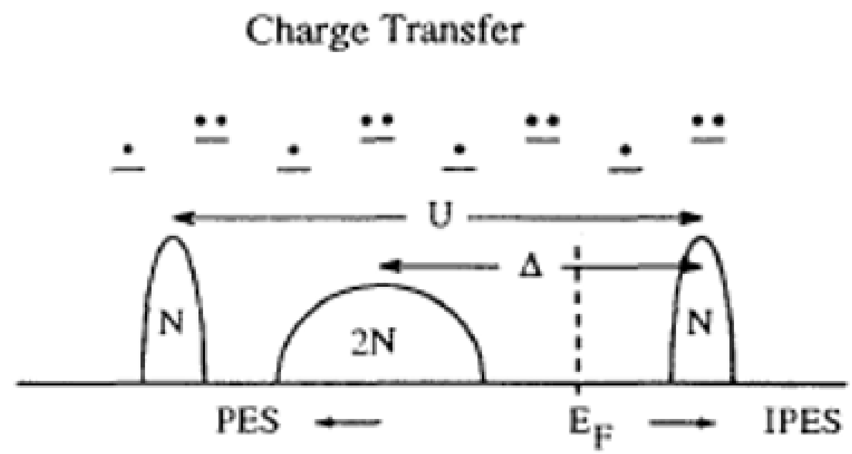


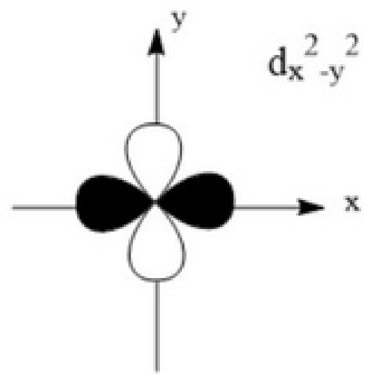


Meinders *et al*. PRB **48**, 3916 (1993)

"Ionic" limiting cases with manageable sign problem



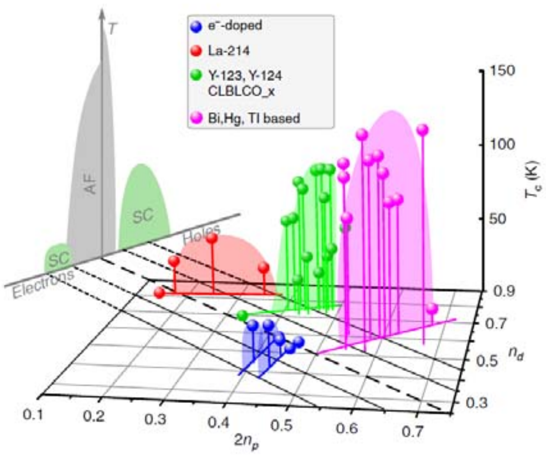




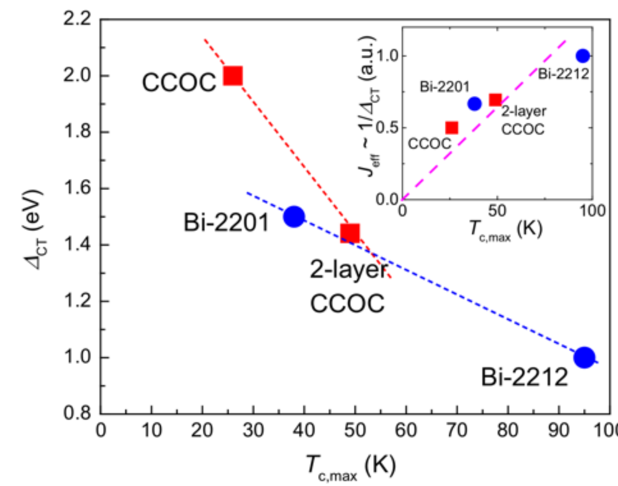
d-wave Superconductivity

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

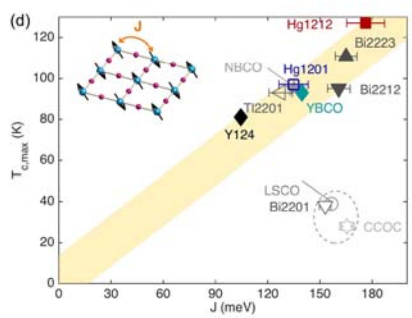
Three experimental observations on optimizing T_c



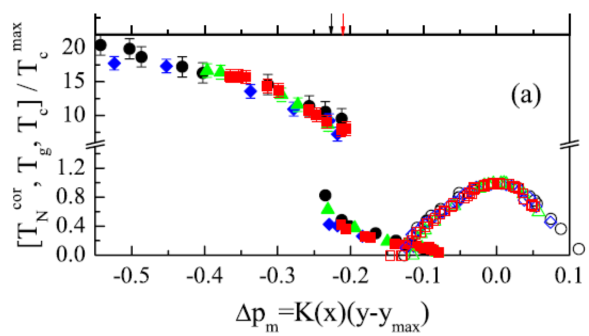
Rybicki, … Haase,
Nat. Comm. 7, 11413
(2016)



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

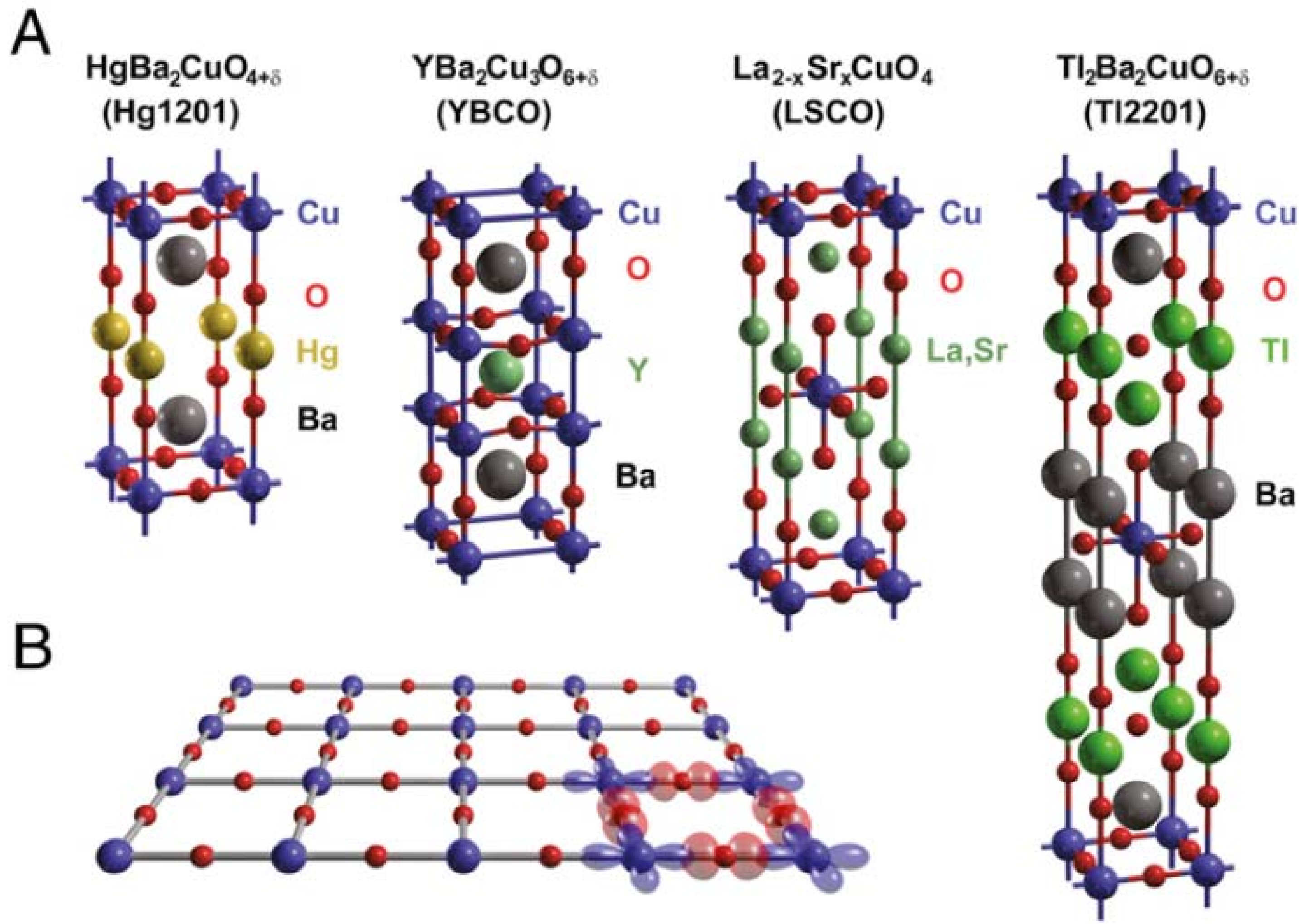


Lichen Wang, *et al.*
arXiv 2011.05029

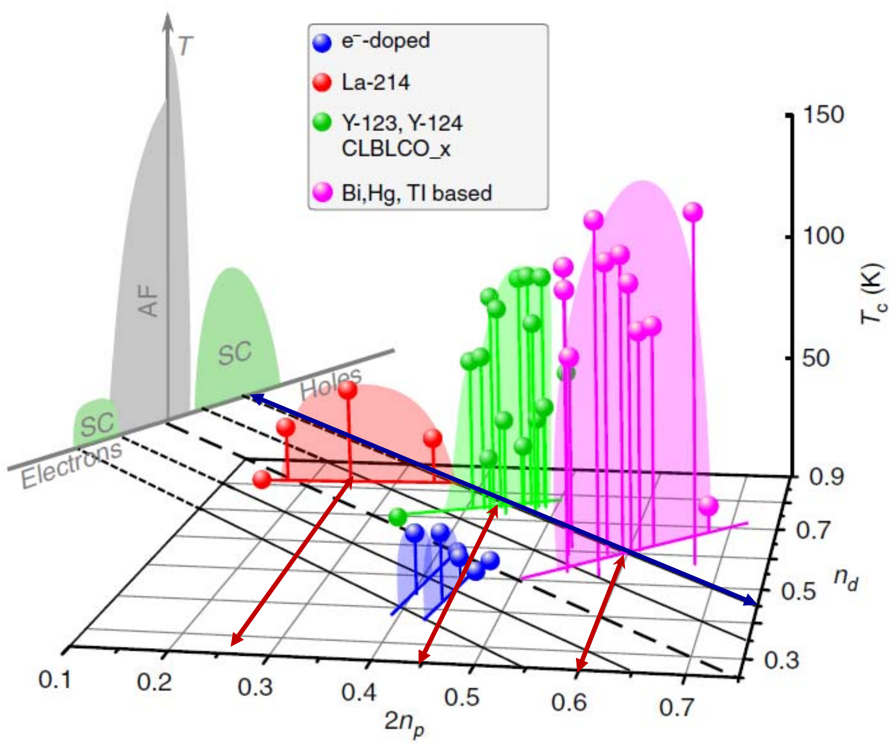


A. Keren New J. Phys. **11** 065006

There are different kinds of cuprates : All with CuO_2 planes



#1 Optimizing T_c with oxygen hole content

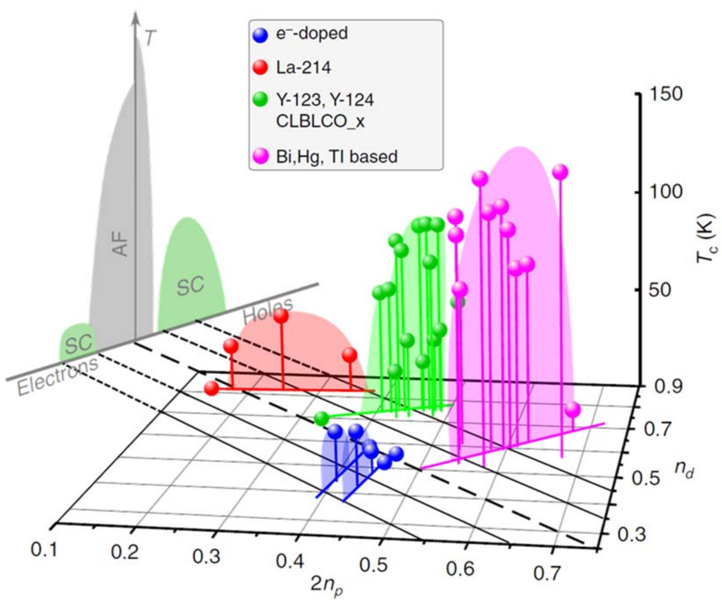


Rybicki,,, Haase, Nat. Comm. 7, 11413 (2016)

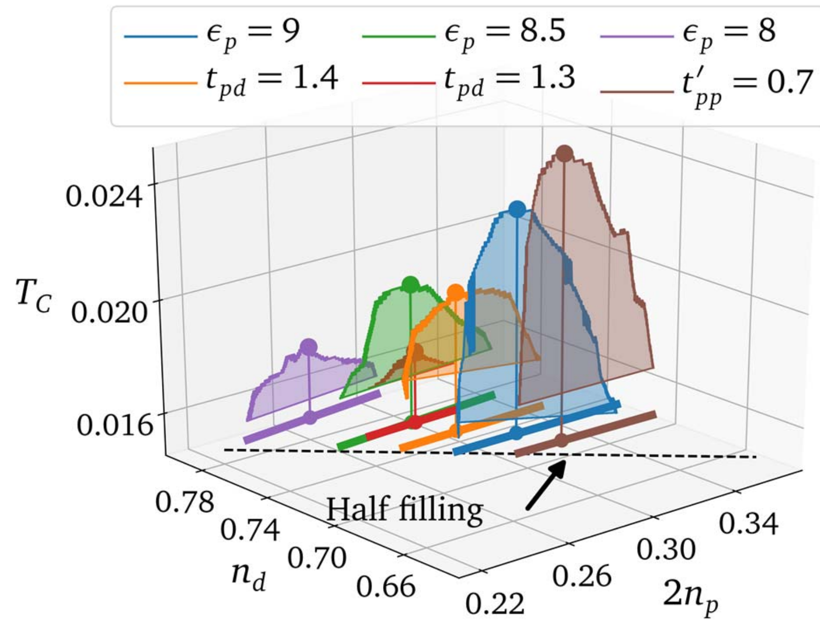
Results

Critical Temperature

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

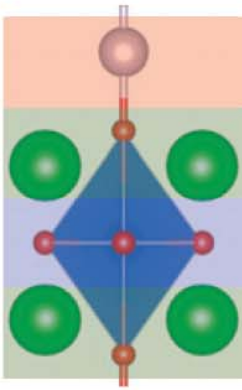


D. Rybicki et al. "Perspective on the phase diagram of cuprate high-temperature superconductors," Nature Communications, vol. 7, p. 11413, 2016



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

Optimizing T_c

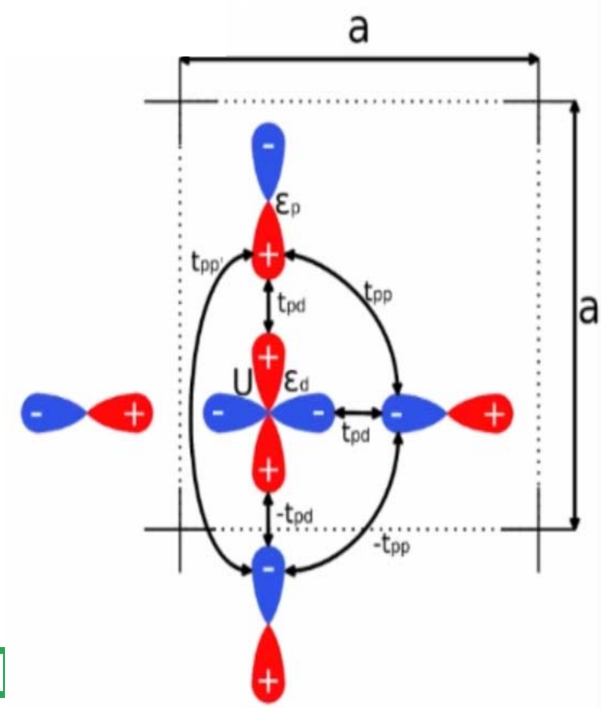


	charge	dopants	structure	hamiltonian
HgO_δ	balances -2 charge	supplies	harbors dopants	tunes chemical potential
BaO	neutral	inert	protects CuO_2 from disorder	tunes in-plane t, t', U
CuO_2	-2 charge/u.c.	accepts	roughly sets lattice const.	superconducts
BaO		(same as other CaS layer)		

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

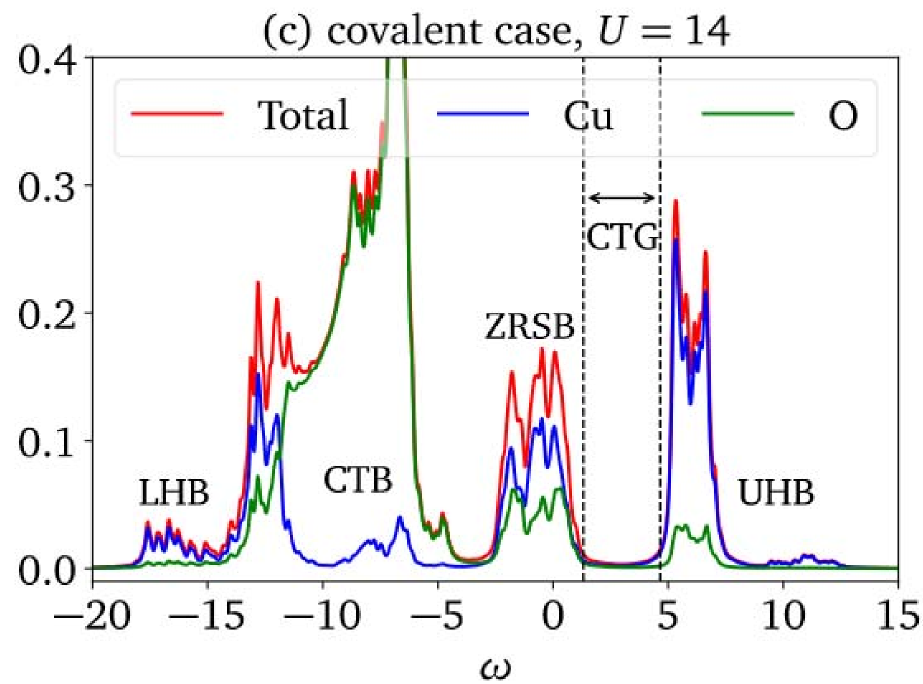
Electronic structure

	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



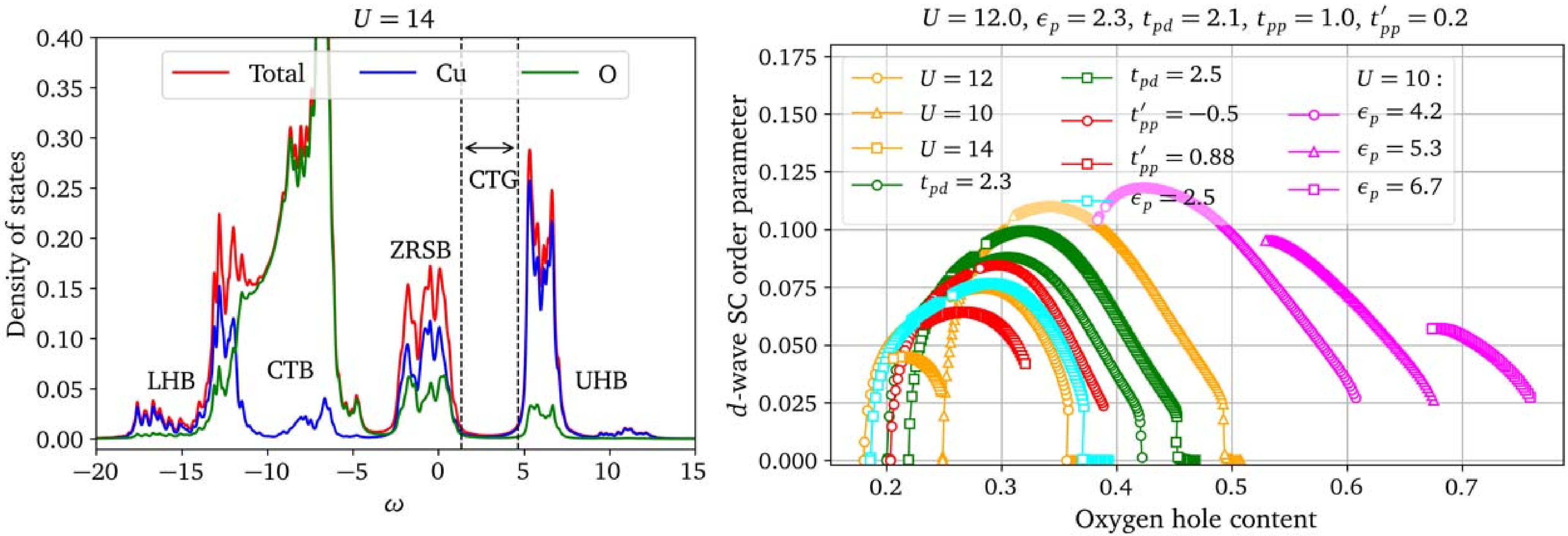
Weber, Yee, Haule, Kotliar, EPL 100, 2012

Density of states



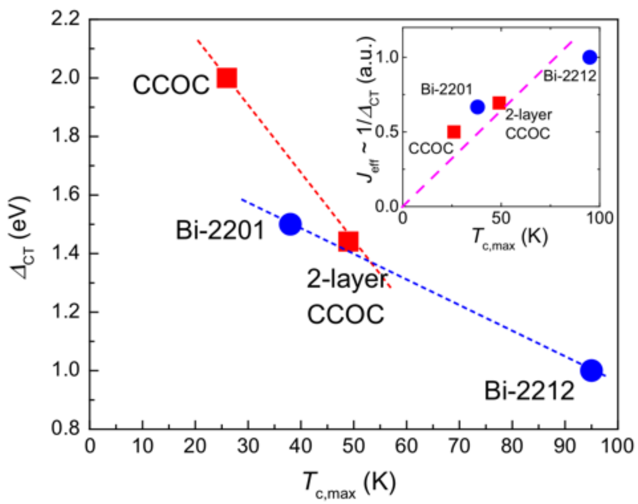
- $\varepsilon_p - \varepsilon_d = 2.3$, $t_{pd} = 2.1$, $t_{pp} = 1.0$, $t'_{pp} = 0.2$

$T = 0$ superconducting domes for the covalent model

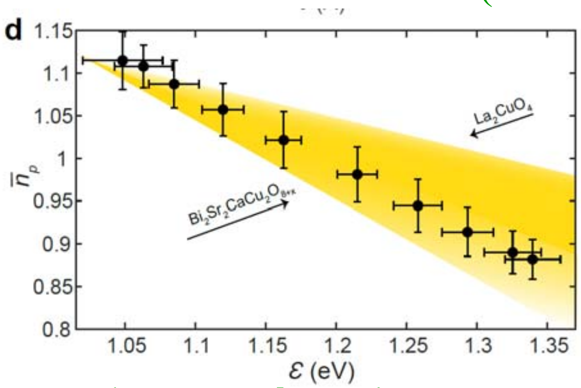


Kowalski, Dash, Sémon, Sénéchal, A-M.T.
PNAS **118** (40) e2106476118 (2021)

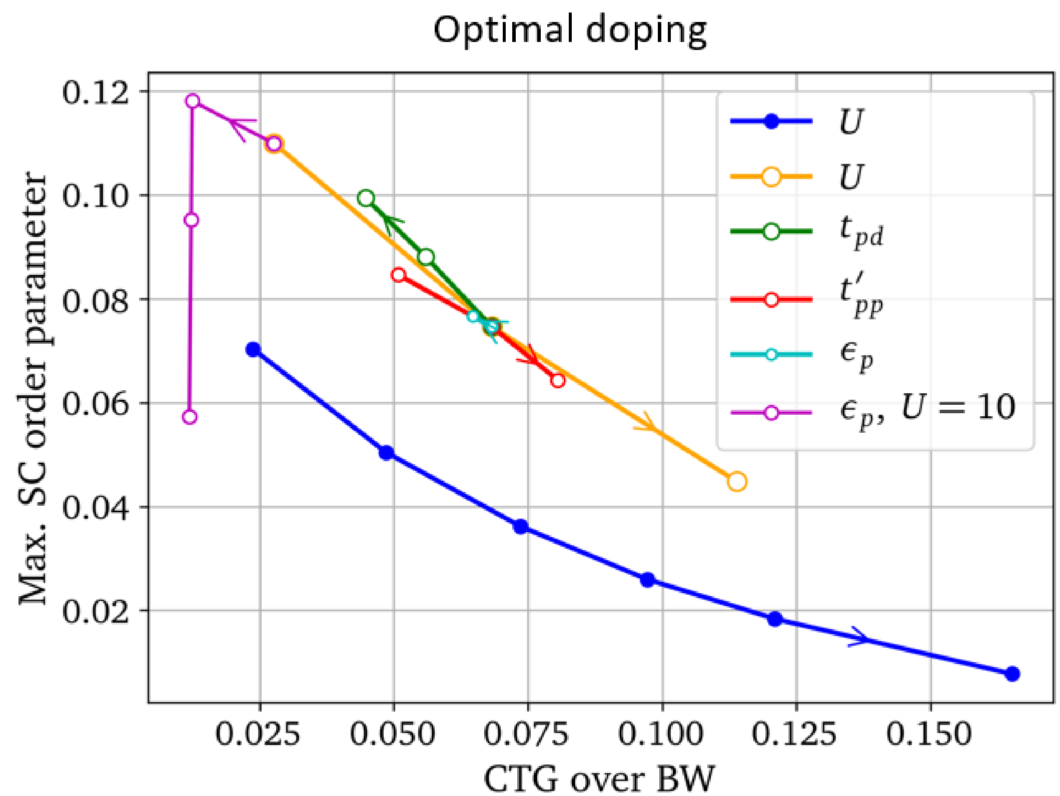
#2 Optimizing T_c with CT gap Δ (Oxygen as a witness)



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

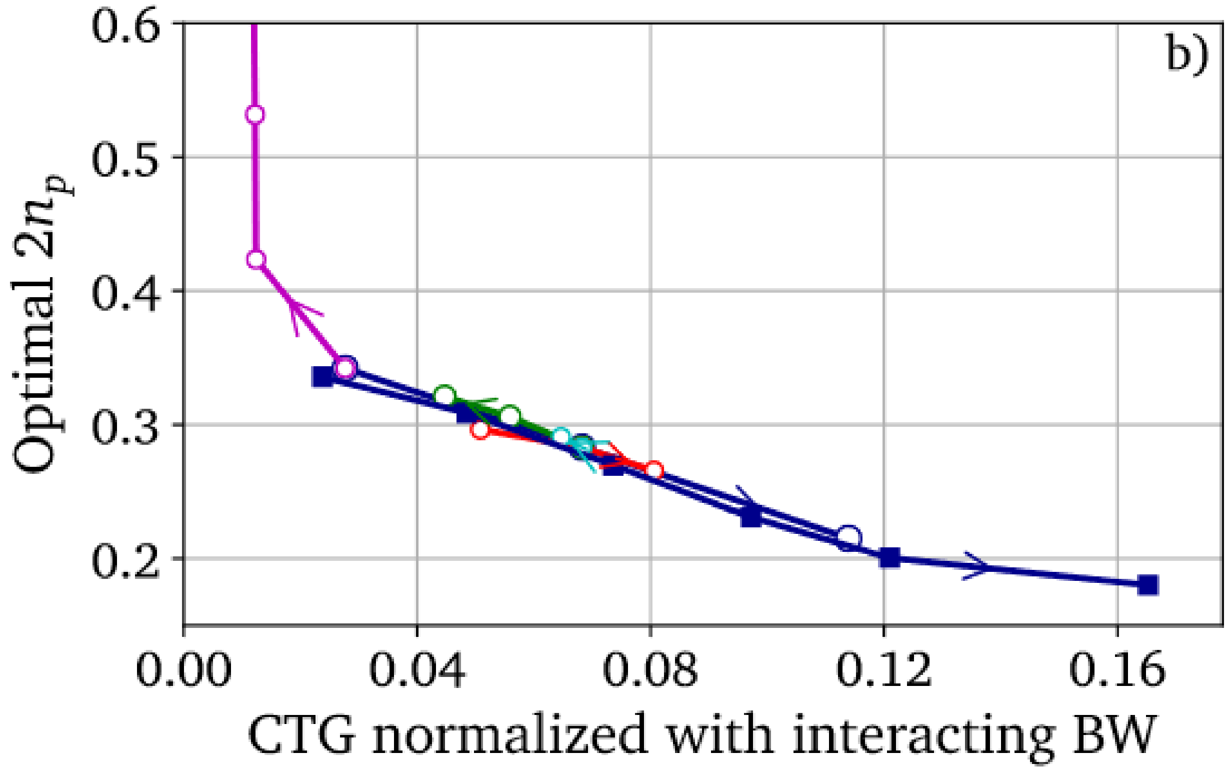


O'Mahony *et al.* arXiv:2108.03655



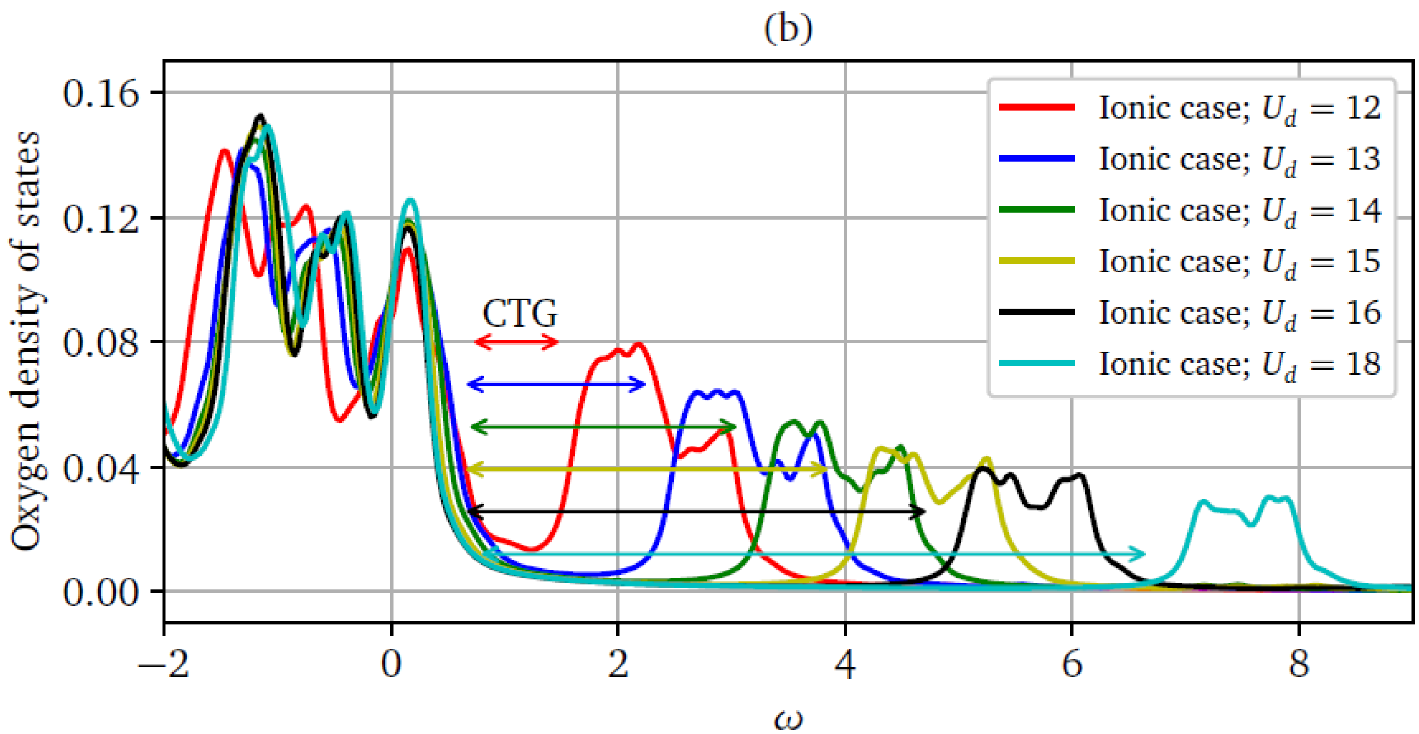
Kowalski, Dash, Sémon, Sénéchal, A-M.T.
PNAS **118** (40) e2106476118 (2021)

Charge-transfer gap, oxygen hole content



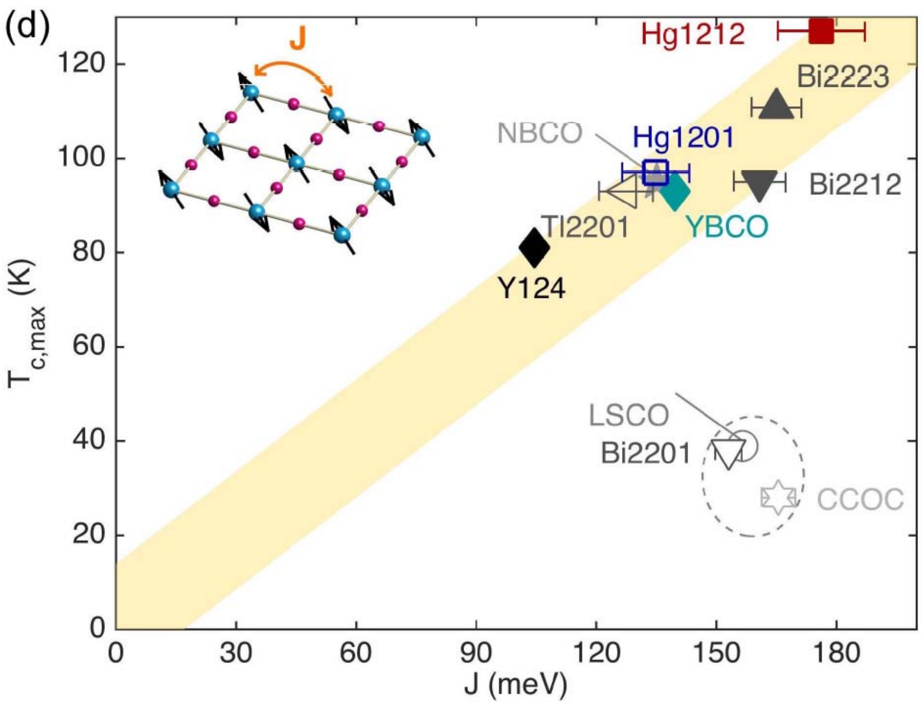
Kowalski, Dash, Sémon, Sénéchal, A-M.T.
PNAS **118** (40) e2106476118 (2021)

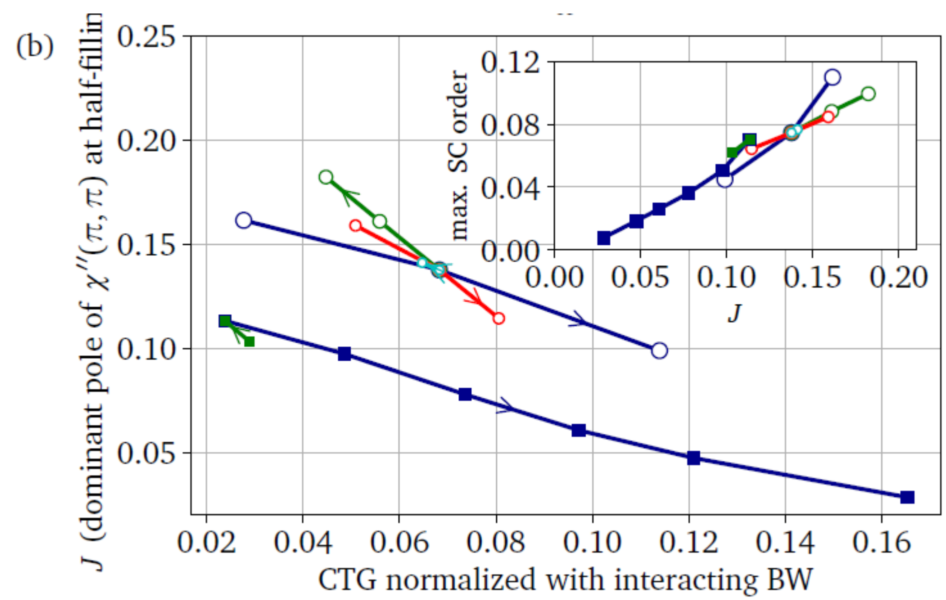
Charge transfer gap and oxygen hole content : Oxygen as a witness



Copper pairing mechanism : superexchange

#3 Optimizing T_c with superexchange





Lichen Wang, *et al.* arXiv 2011.05029

$J = 4t^2/U$

D. Sénéchal

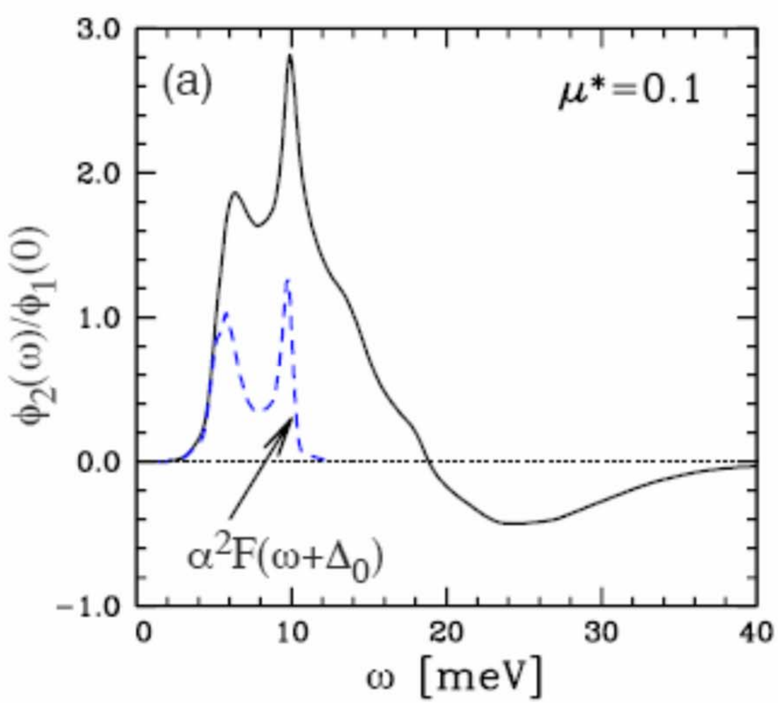
Bumsoo Kyung

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)

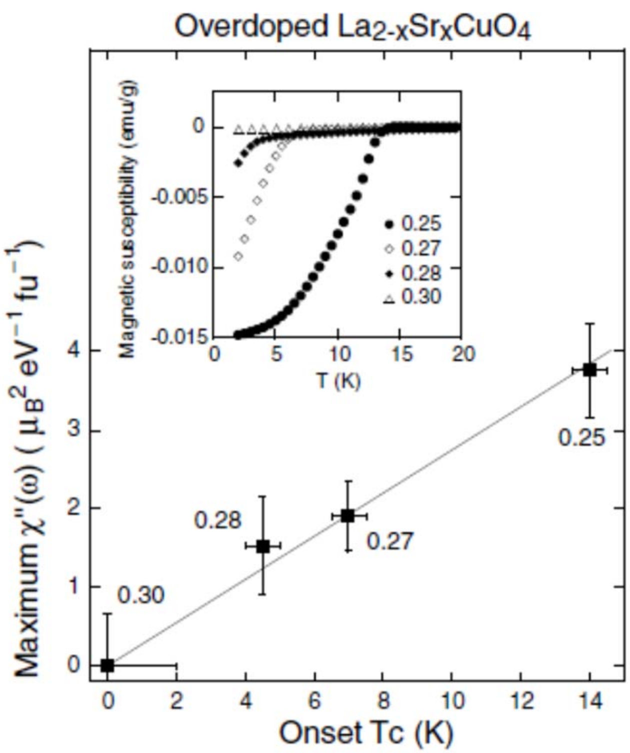
Im Σ_{an} and electron-phonon in Pb

Maier, Poilblanc, Scalapino, PRL (2008)

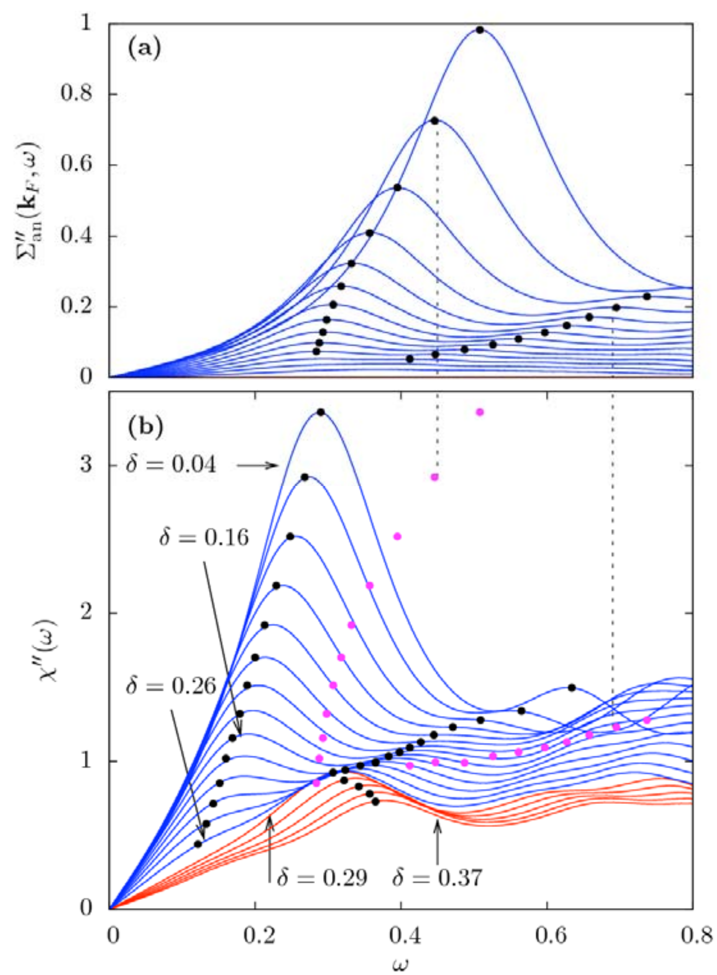


The glue CDMFT 2x2, T=0

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

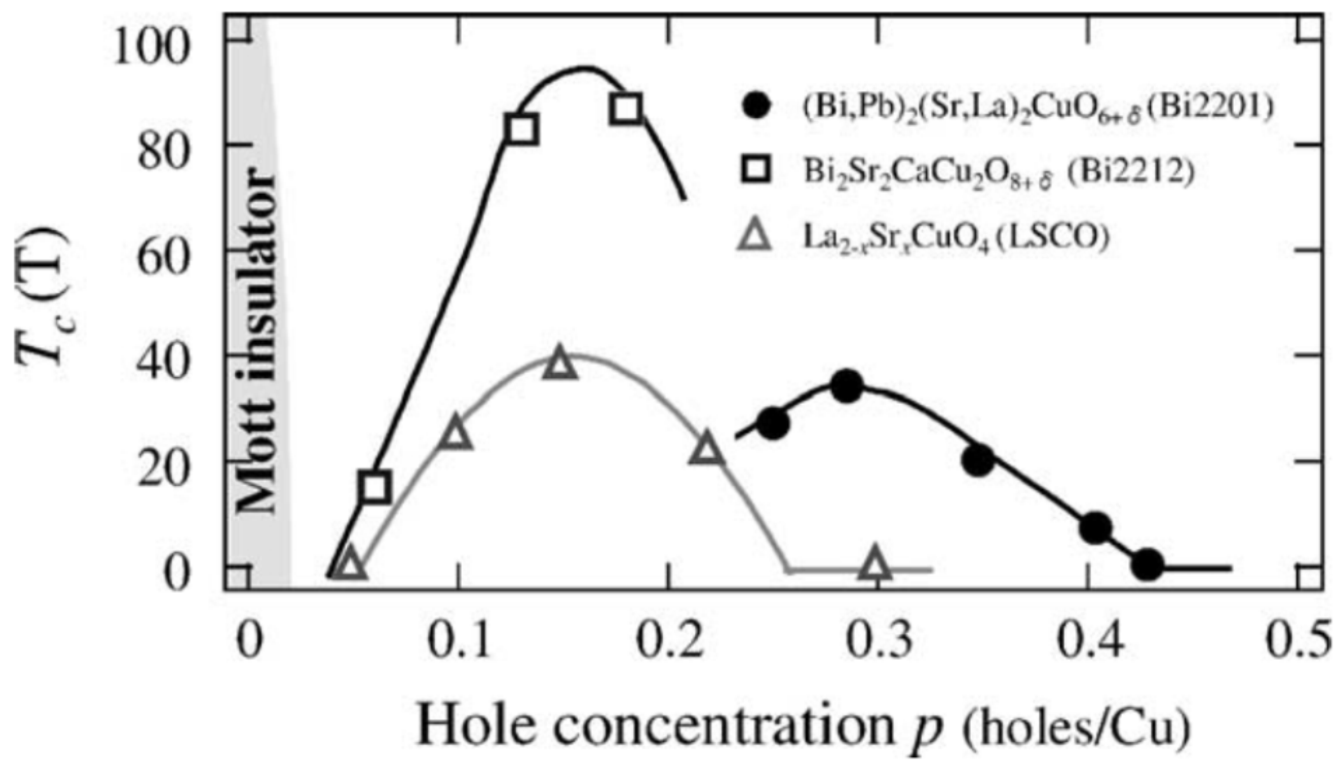


Wakimoto … Birgeneau PRL (2004)



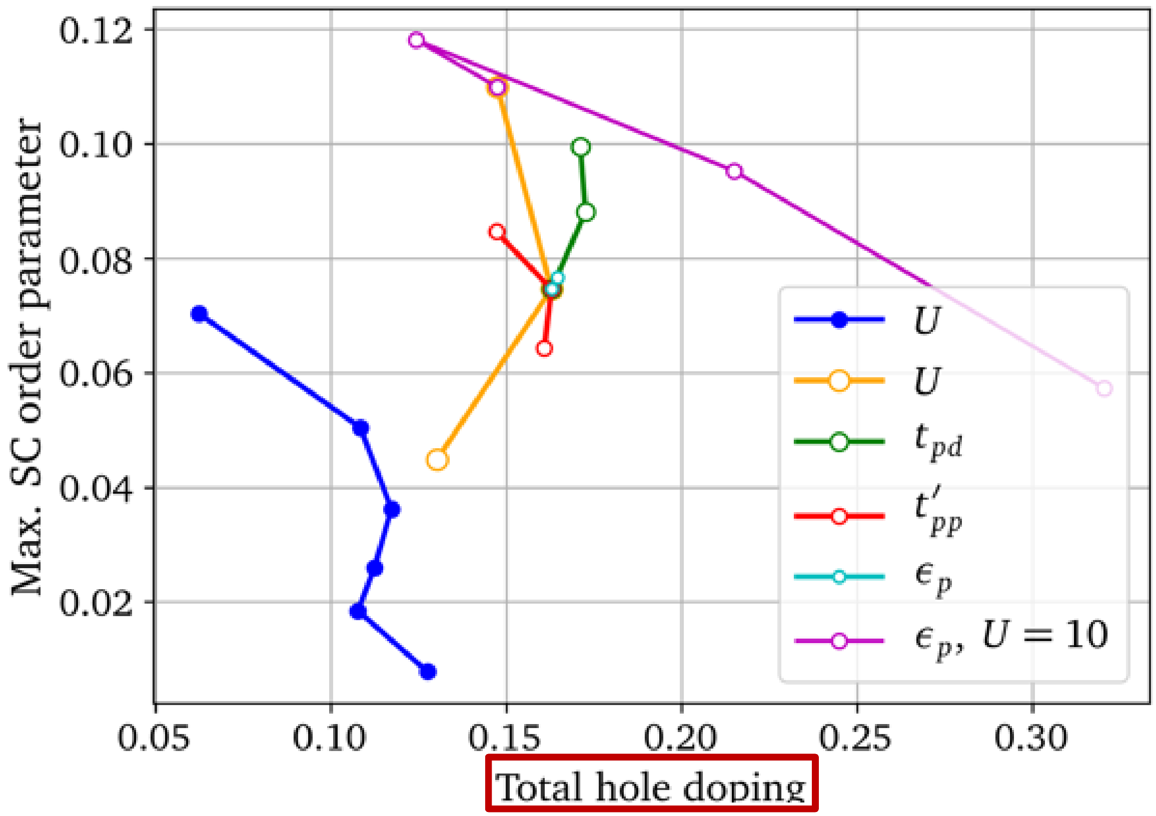
Bonus

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)

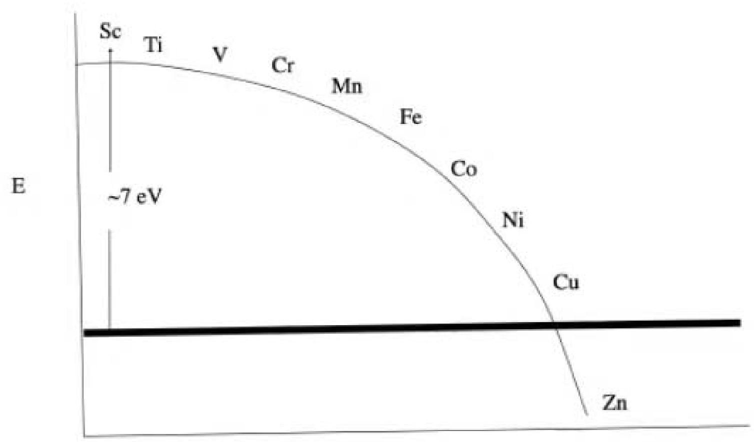
Bonus: total hole doping does not explain max order parameter for the two models



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

Optimizing Tc

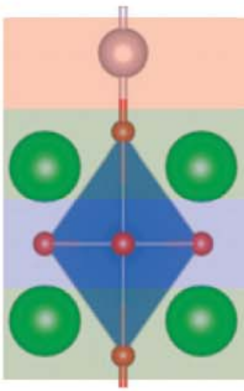
- Spin ½
- One band
- Two-dimensions
- Strong covalency between chalchogen and transition metal.
  - Chalcogen screens U
- Charge-transfer gap just opening (intermediate interactions).
- Large J at half-filling
- … and more

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



	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)	

$$Hg(CaS)_2CuO_2$$

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