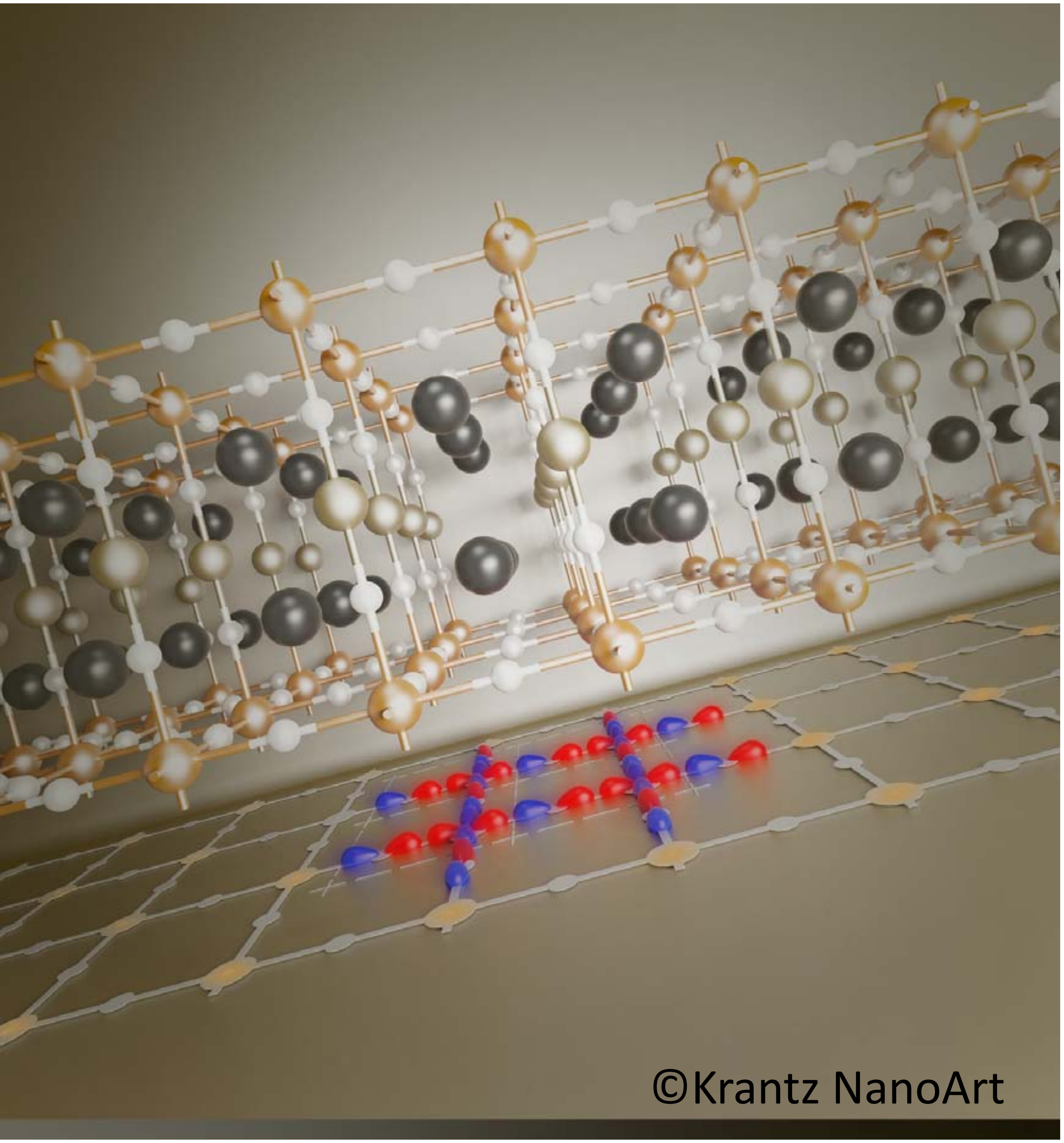

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CRSNG NSERC

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Fonds de recherche Nature et technologies Québec

Superconductivity in the three-band model of cuprates vs experiments

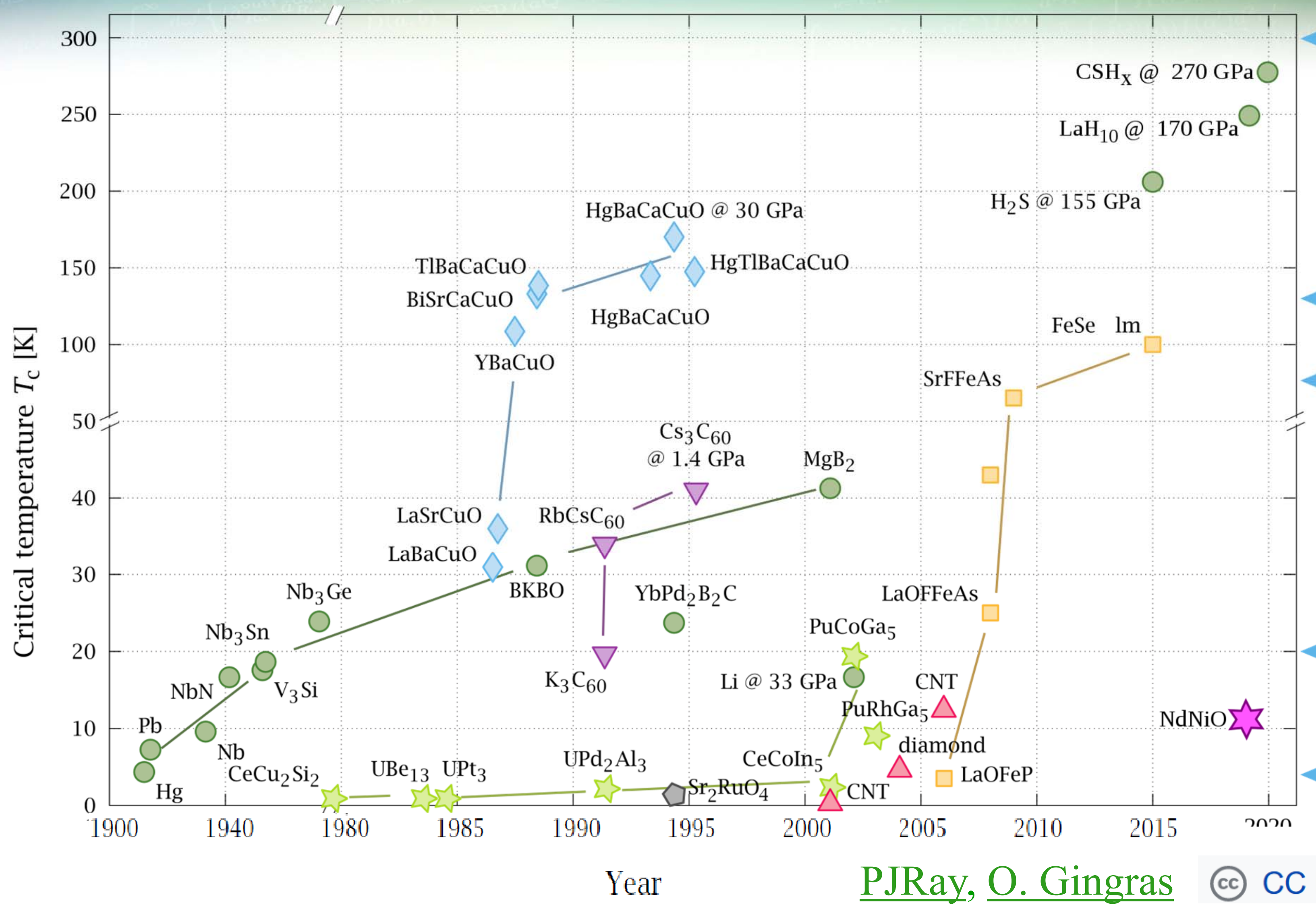
André-Marie Tremblay
Université de Sherbrooke
Institut quantique

CORPES22 Virtual meeting, July 11, 2022

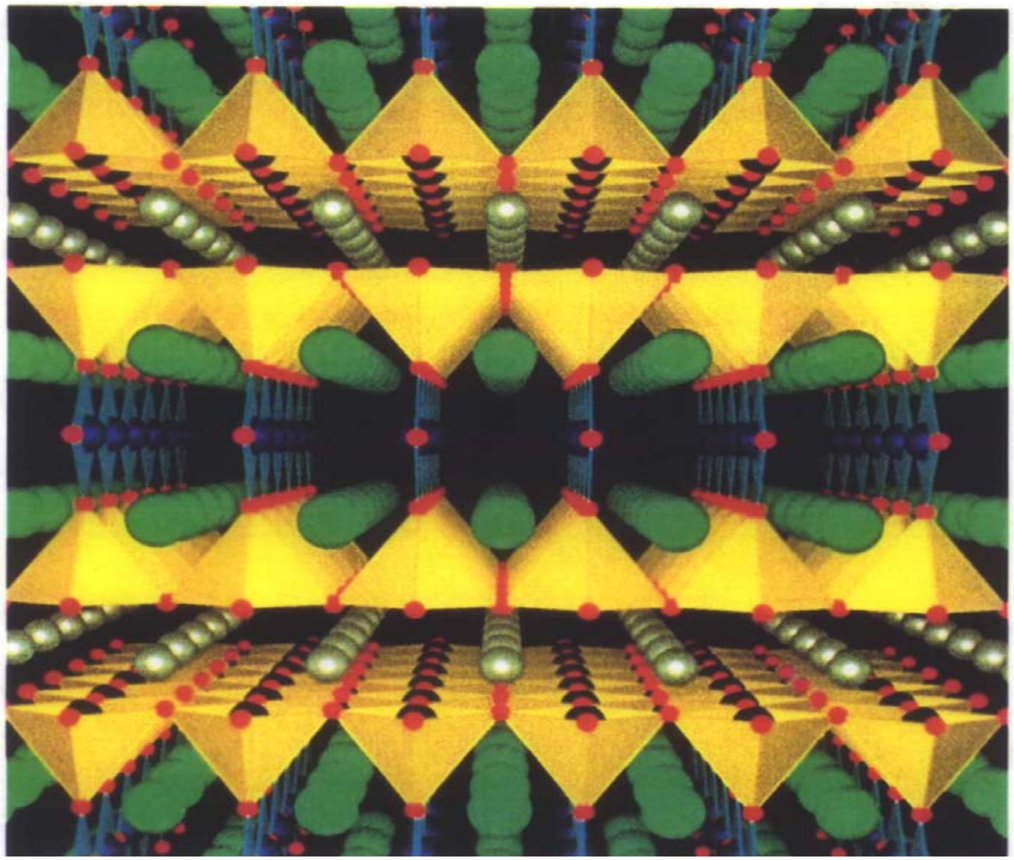
Institut quantique

Université de Sherbrooke

USHERBROOKE.CA/IQ


Critical temperature T_c [K]
Year
300
250
200
150
100
50
40
30
20
10
0
1900
1940
1980
1985
1990
1995
2000
2005
2010
2015
2020
Hg
Pb
Nb
NbN
V_3Si
Nb_3Sn
Nb_3Ge
$CeCu_2Si_2$
UBe_{13}
UPt_3
UPd_2Al_3
LaBaCuO
LaSrCuO
YBaCuO
BiSrCaCuO
TlBaCaCuO
HgBaCaCuO
HgBaCaCuO @ 30 GPa
HgTlBaCaCuO
BKBO
K_3C_{60}
$RbCsC_{60}$
Cs_3C_{60}
@ 1.4 GPa
$YbPd_2B_2C$
Sr_2RuO_4
MgB_2
$CeCoIn_5$
CNT
$PuCoGa_5$
Li @ 33 GPa
$PuRhGa_5$
CNT
diamond
LaOFeP
LaOFFeAs
SrFFeAs
FeSe
H_2S @ 155 GPa
LaH_{10} @ 170 GPa
CSH_x @ 270 GPa
NdNiO

Cuprates : Atomic structure



Outline

- Method
- 3-band Model

- Three experiments that tell us how to optimize Tc.
- Pairing mechanism
- Bonus

- Conclusion

Method : Model building

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

Method
Solving the models

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

Method

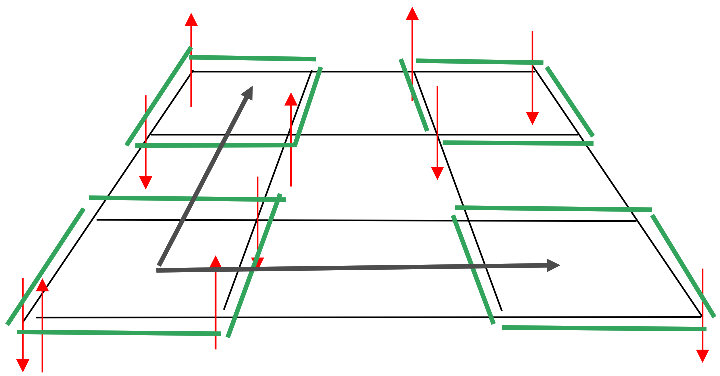
Cluster generalization of
Dynamical Mean-Field Theory : DMFT

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

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

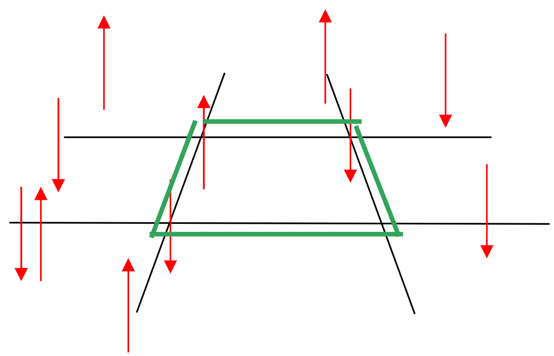
Localized and delocalized pictures C-DMFT

Delocalized



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

Localized



$$G_{ij} = \int \frac{d^d\tilde{k}}{(2\pi)^d} \left(\frac{1}{(i\omega_n+\mu)I-\varepsilon(\tilde{k})-\Gamma_O(i\omega_n)-\Sigma(i\omega_n)} \right)_{ij} \quad (G^{-1})_{ij} = (G_0^{-1})_{ij} - \Sigma_{ij}$$

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

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

Impurity solvers

Impurity solver : continuous-time quantum Monte Carlo

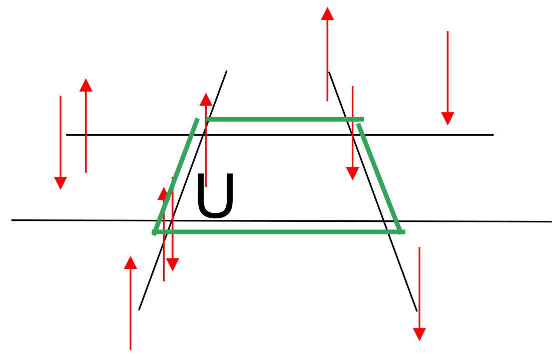
$$Z = \int \mathcal{D}[\psi^\dagger, \psi]\, e^{-S_c - \int_0^\beta d\tau \int_0^\beta d\tau' \sum_{\mathbf{K}} \psi^\dagger_{\mathbf{K}}(\tau) \Delta_{\mathbf{K}}(\tau,\tau') \psi_{\mathbf{K}}(\tau')}$$

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**

Impurity solver (Exact diagonalisation)



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

QCM David Sénéchal

Some groups using these methods for cuprates

- Europe:
  - Georges, Parcollet, Ferrero, Civelli, Fratino (Paris)
  - Sordi (London), 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 of the method: advantages and limitations

+ 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

Three-band (Emery VSA) Hubbard model

Sidhartha Dash

Nicolas Kowalski

Patrick Sémon

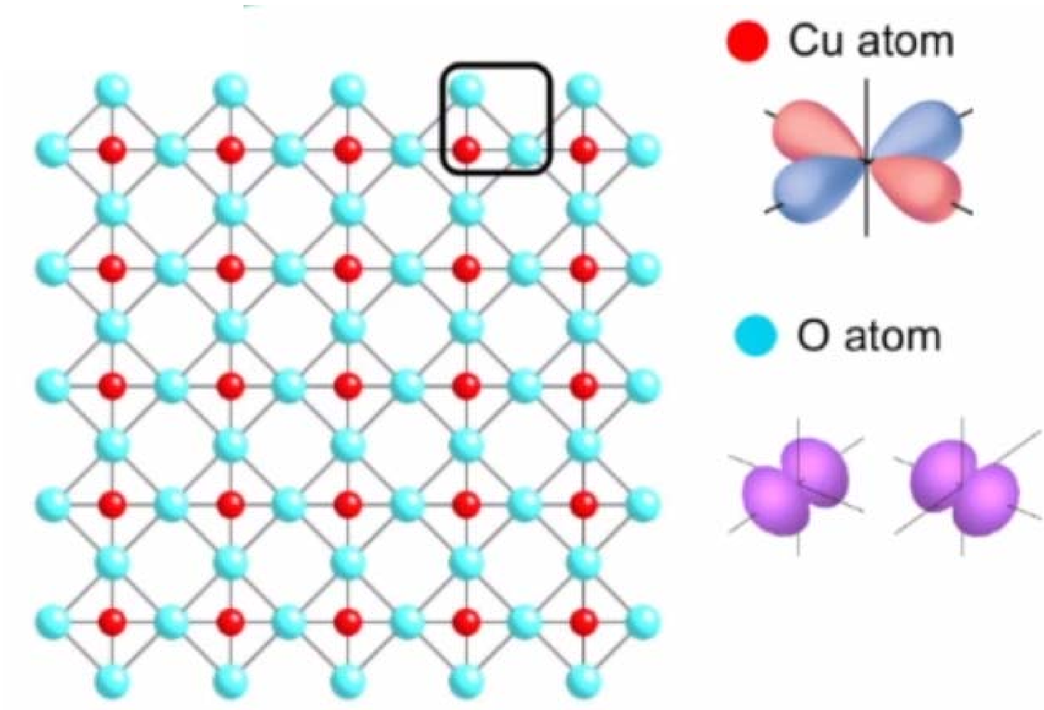
David Sénéchal

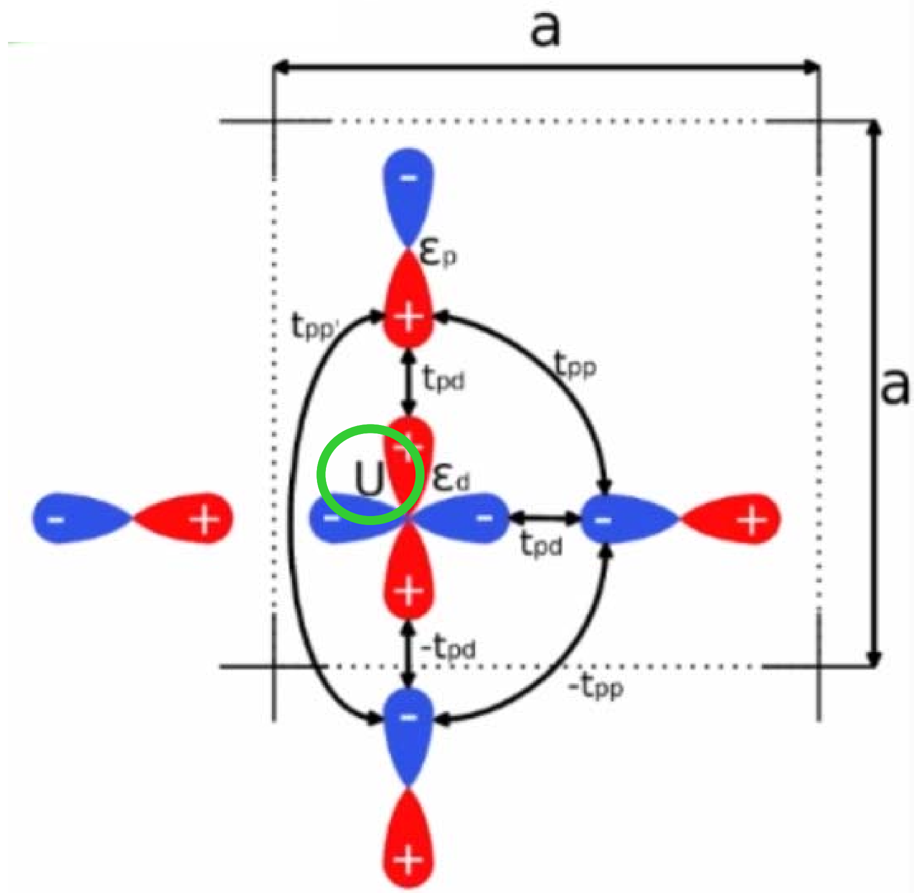
V. J. Emery, Phys. Rev. Lett. **58**, 2794 (1987)

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

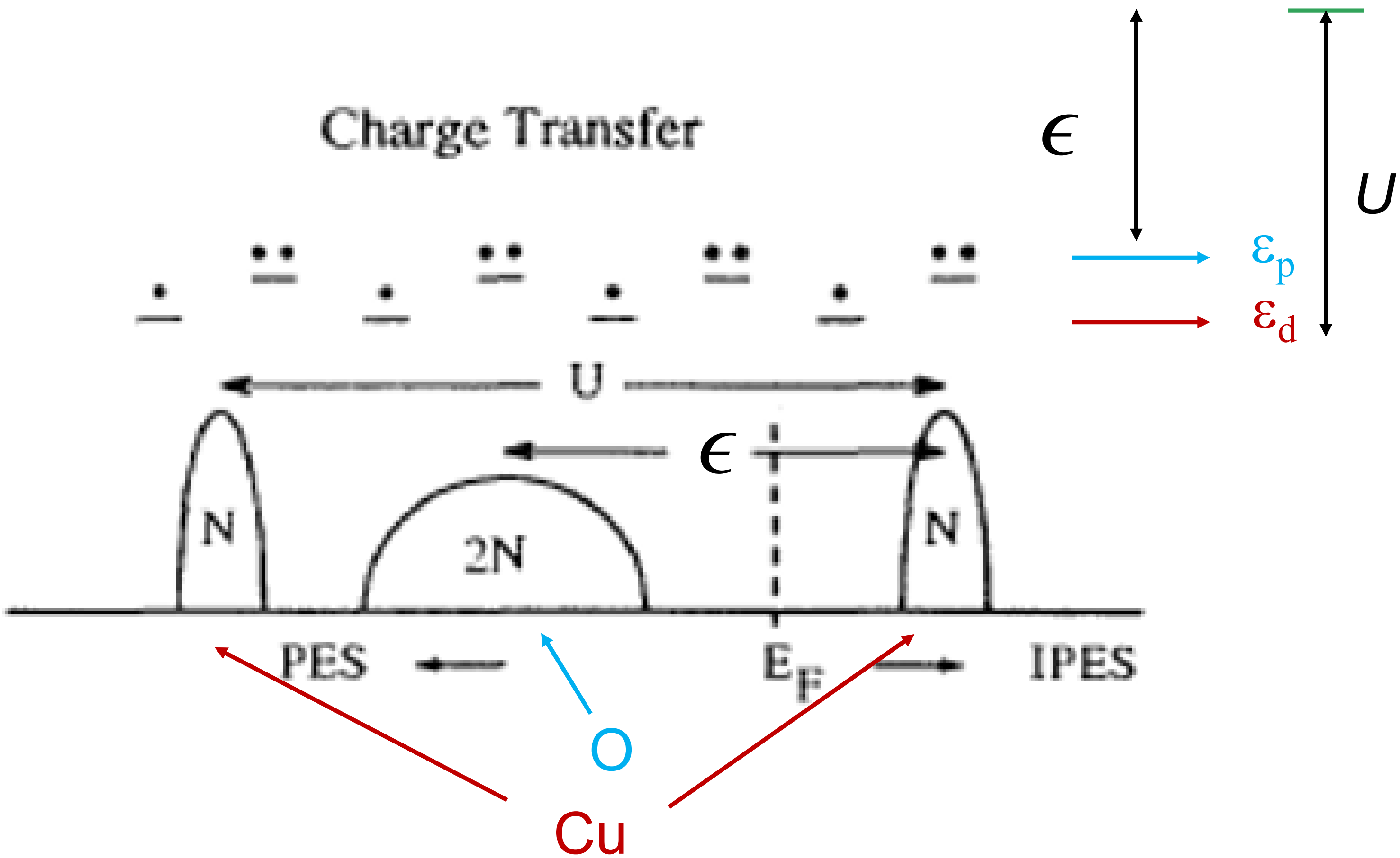
PNAS **118** (40) e2106476118 (2021)

Copper and oxygen planes



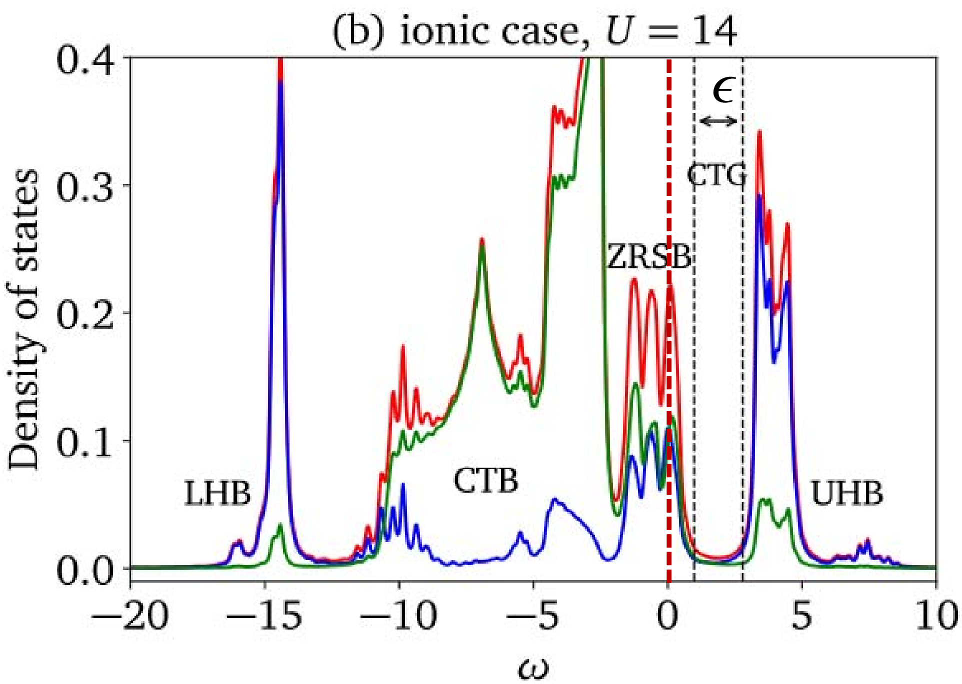


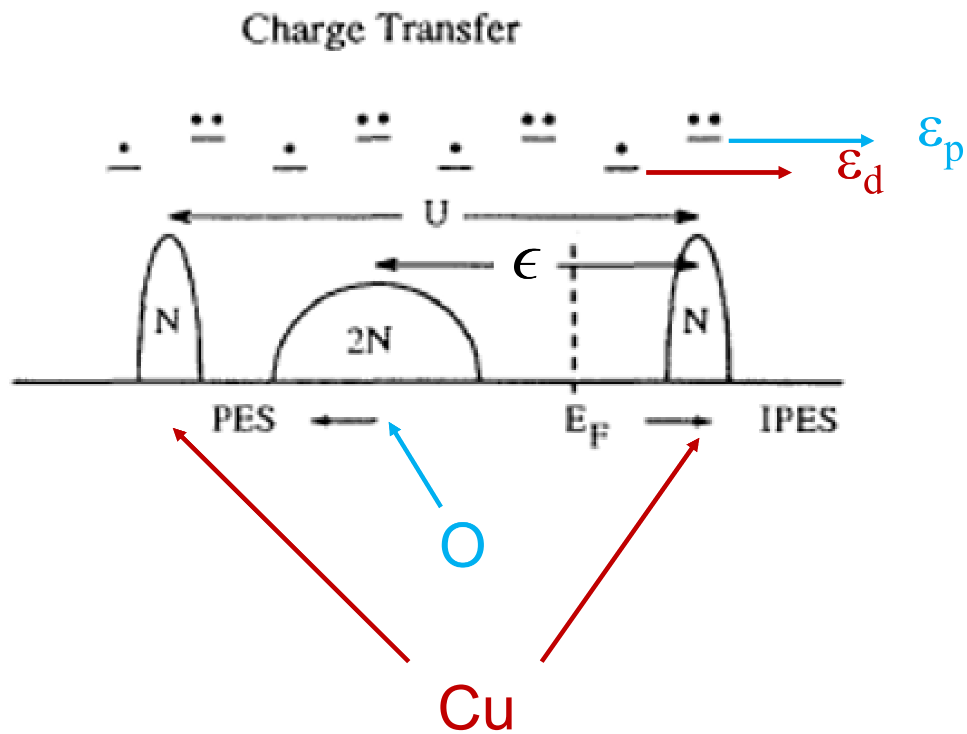
Cartoon of the charge transfer insulator



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

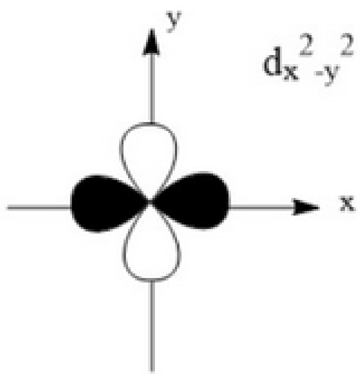
"Ionic" limiting cases with manageable sign problem





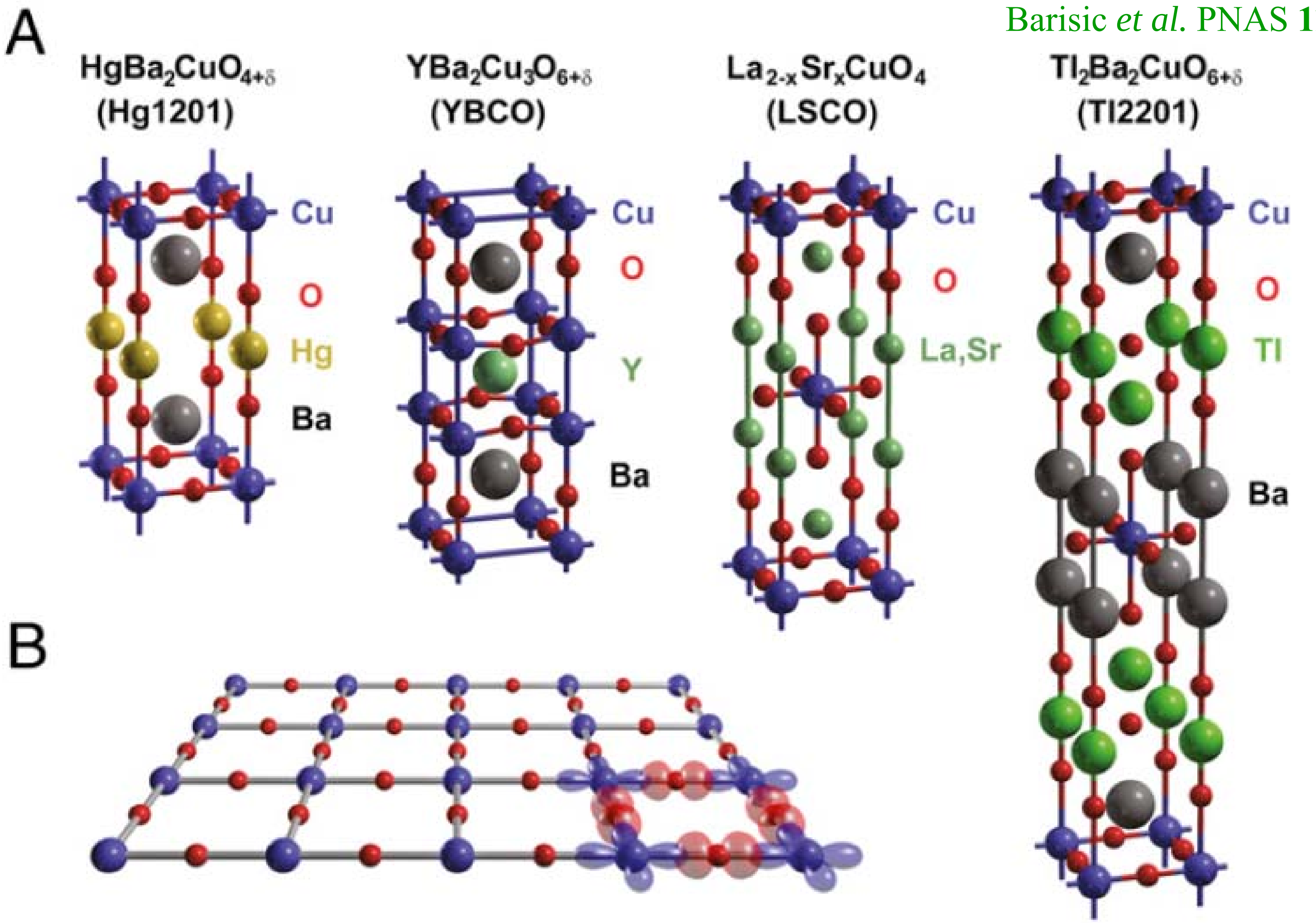
Meinders *et al.* PRB **48**, 3916 (1993)

d-wave Superconductivity

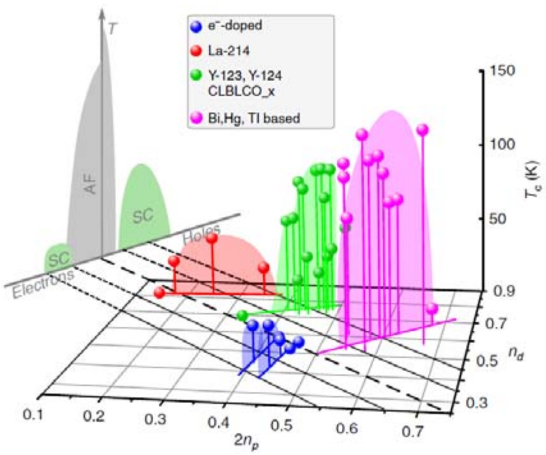


There are different kinds of cuprates : All with CuO_2 planes

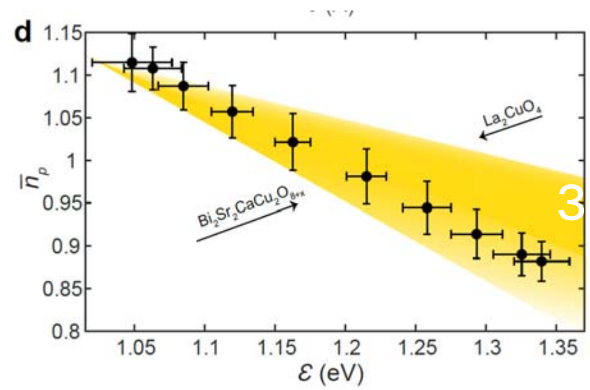
Barisic *et al.* PNAS **110**, 12235 (2013)



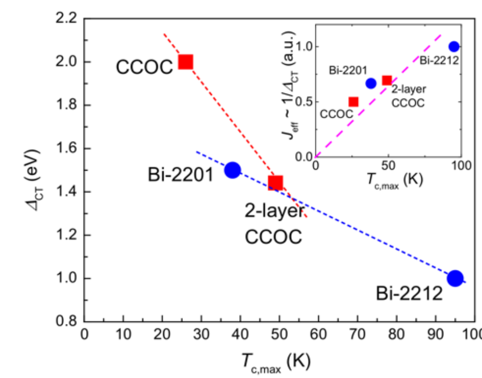
Three experimental observations on optimizing T_c



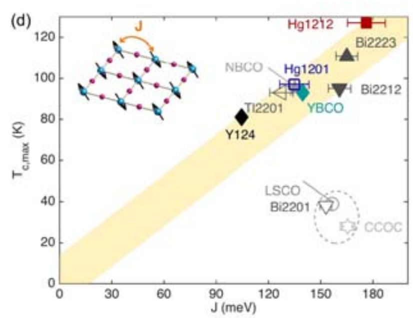
Rybicki, … Haase,
Nat. Comm. 7, 11413
(2016)



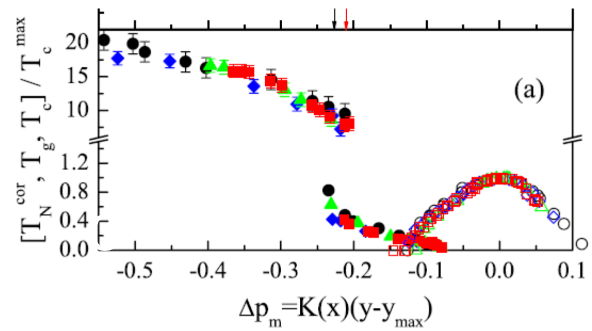
O'Mahony *et al.* arXiv:2108.03655



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



Lichen Wang,
Nat. Comm. **13**, 3163 (2022)



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

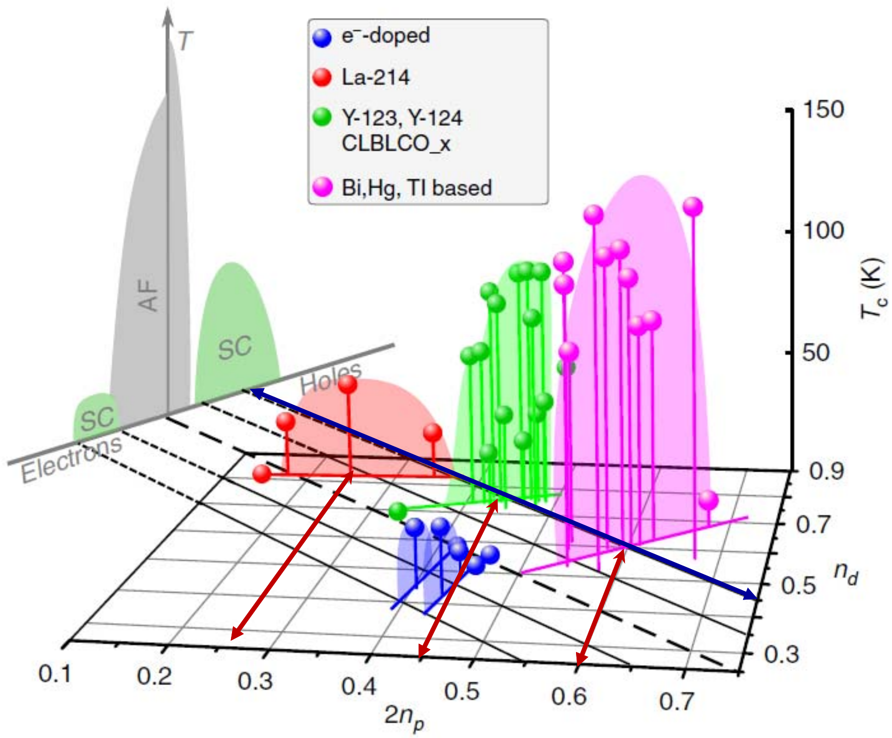
The strategy

The strategy

- Variations in microscopic parameters in Hamiltonian
  - "Ionic" class of models
    - Large value of $\varepsilon_p - \varepsilon_d$
  - "Covalent" class of models
    - Smaller and more realistic value of $\varepsilon_p - \varepsilon_d$

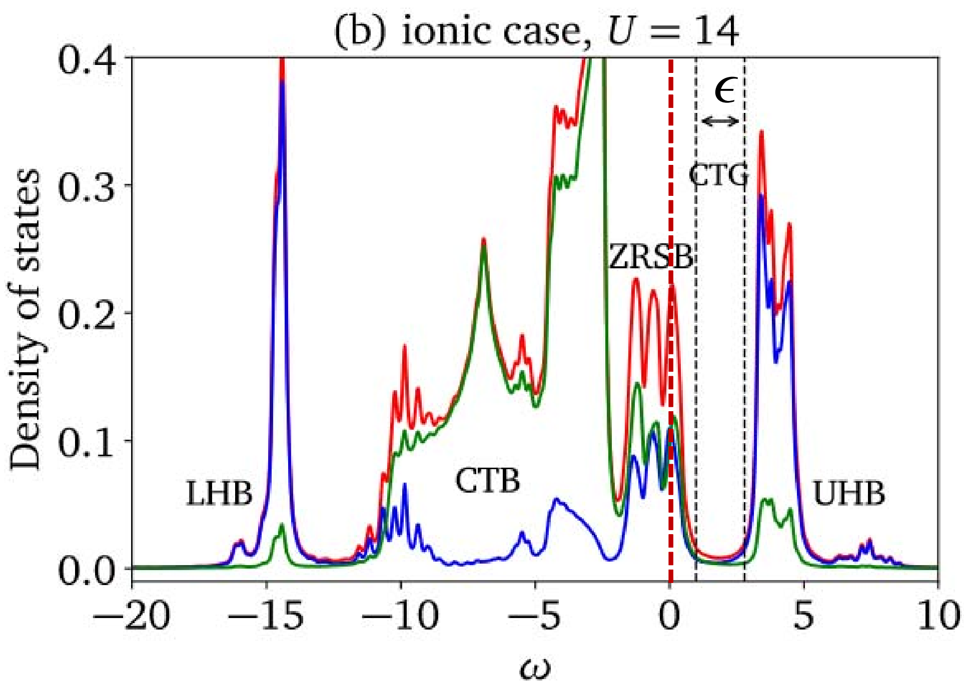
#1 Optimizing T_c with oxygen hole content

#1 Optimizing T_c with oxygen hole content



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

"Ionic" limiting cases with manageable sign problem



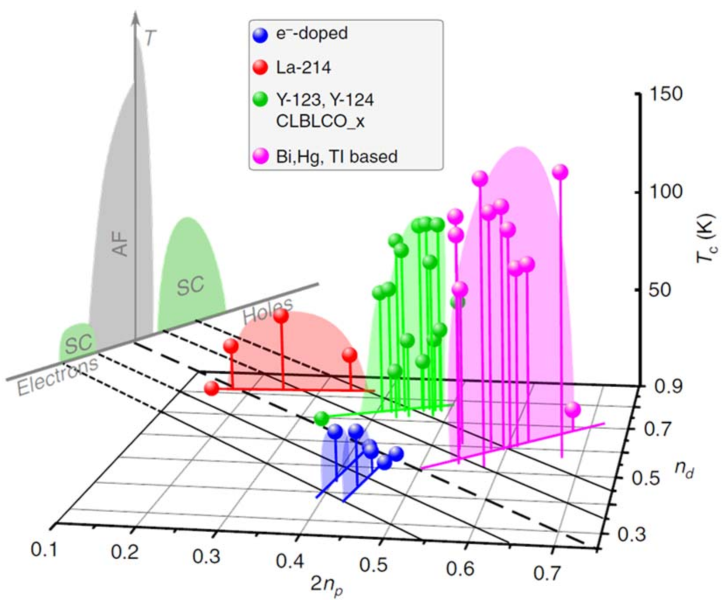
- $\varepsilon_p - \varepsilon_d = 7.0$, $t_{pd} = 1.5$, $t_{pp} = 1.0$, $t'_{pp} = 1.0$

Also, Fratino, Sémon, Sordi, AMT, PRB **93**, 245147 (2016)

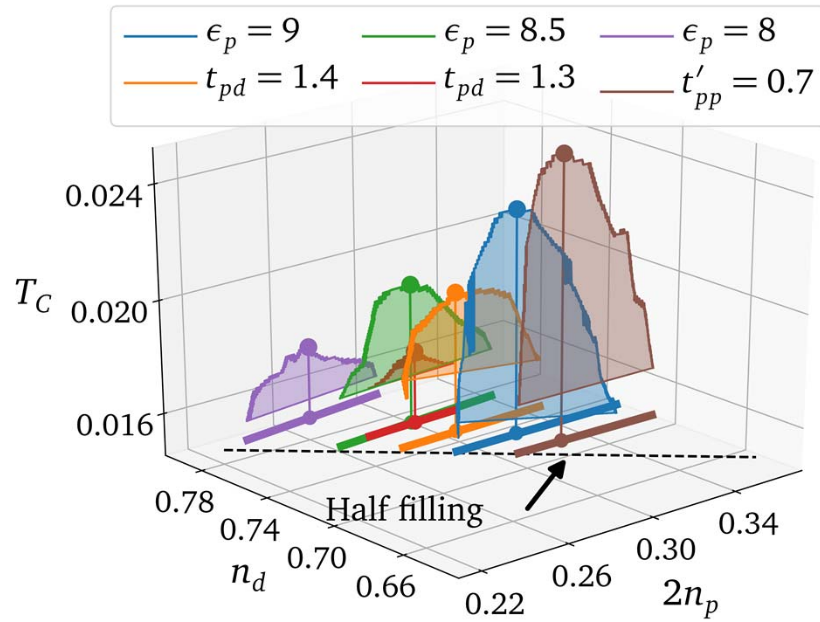
Results

Critical Temperature

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



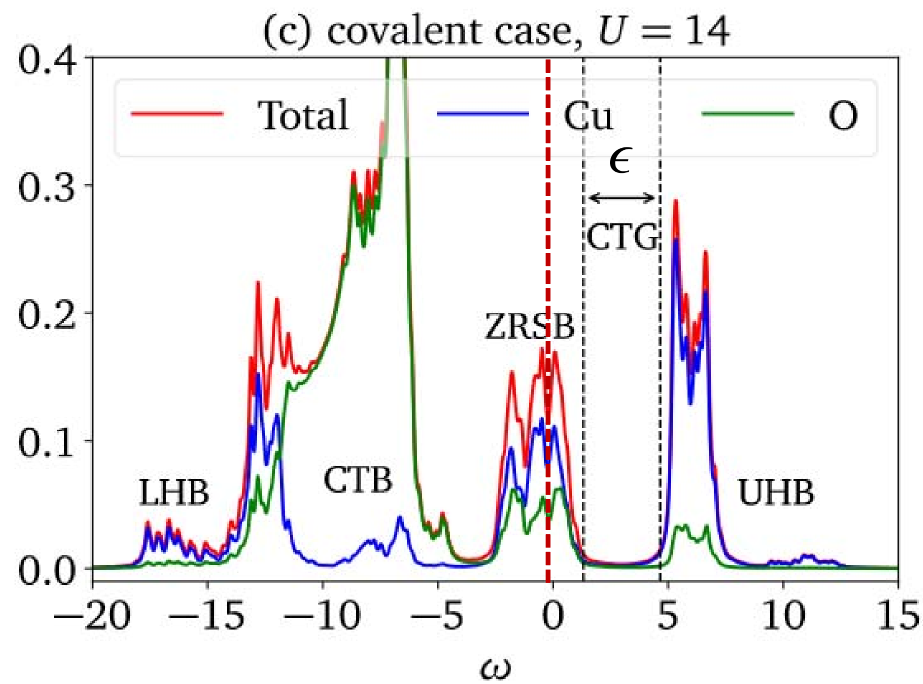
D. Rybicki et al. “Perspective on the phase diagram of cuprate high-temperature superconductors,” Nature Communications, vol. 7, p. 11413, 2016



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

"Covalent" models (*T = 0*)

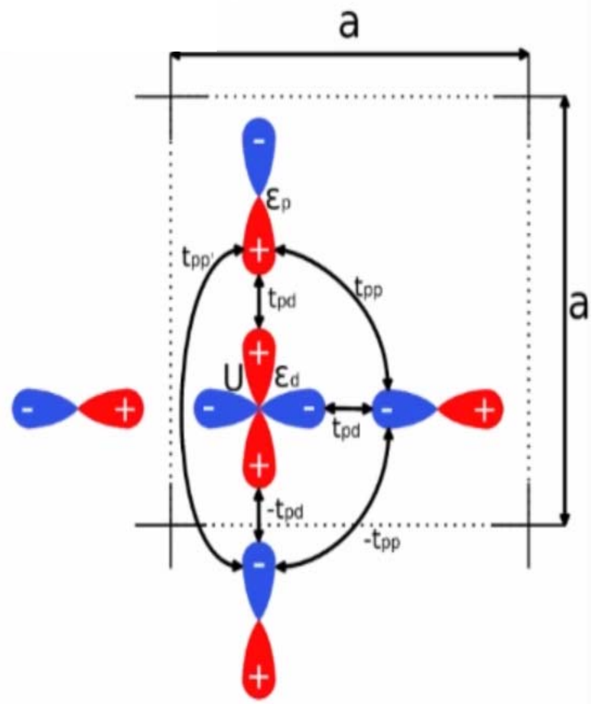
"Realistic"



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

Electronic structure

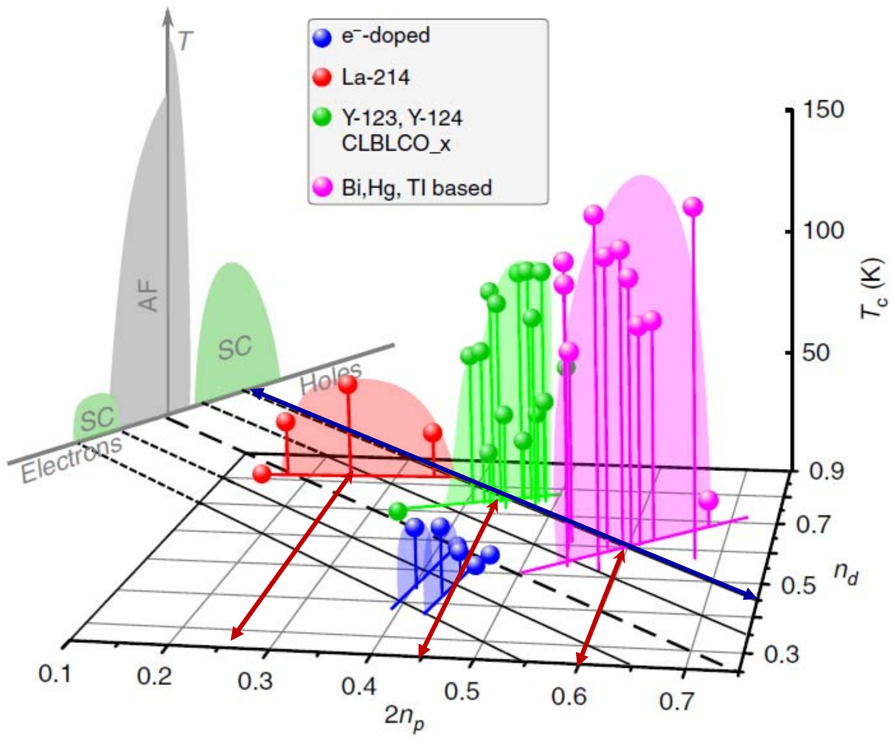
	Compound	$\epsilon_d - \epsilon_p$ (eV)	t_{pd} (eV)	t_{pp} (eV)	$t_{pp'}$ (eV)	t'/t	layers	$d^{\text{apical}}_{\text{Cu-O}}$ (Å)	T_c (K)
(1)	La_2CuO_4	2.61	1.39	0.640	0.103	0.070	1	2.3932	38
(2)	$Pb_2Sr_2YCu_3O_8$	2.32	1.30	0.673	0.160	0.108	2	2.3104	70
(3)	$Ca_2CuO_2Cl_2$	2.21	1.27	0.623	0.132	0.085	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

#1 Optimizing T_c with oxygen hole content



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

T = 0 exact diagonalization solver : order parameter

$$2\hat{\Delta} = \sum_{\langle ij\rangle_x} (d_{i,\uparrow} d_{j,\downarrow} - d_{i,\downarrow} d_{j,\uparrow}) - \sum_{\langle ij\rangle_y} (d_{i,\uparrow} d_{j,\downarrow} - d_{i,\downarrow} d_{j,\uparrow}) + \text{H.c.},$$

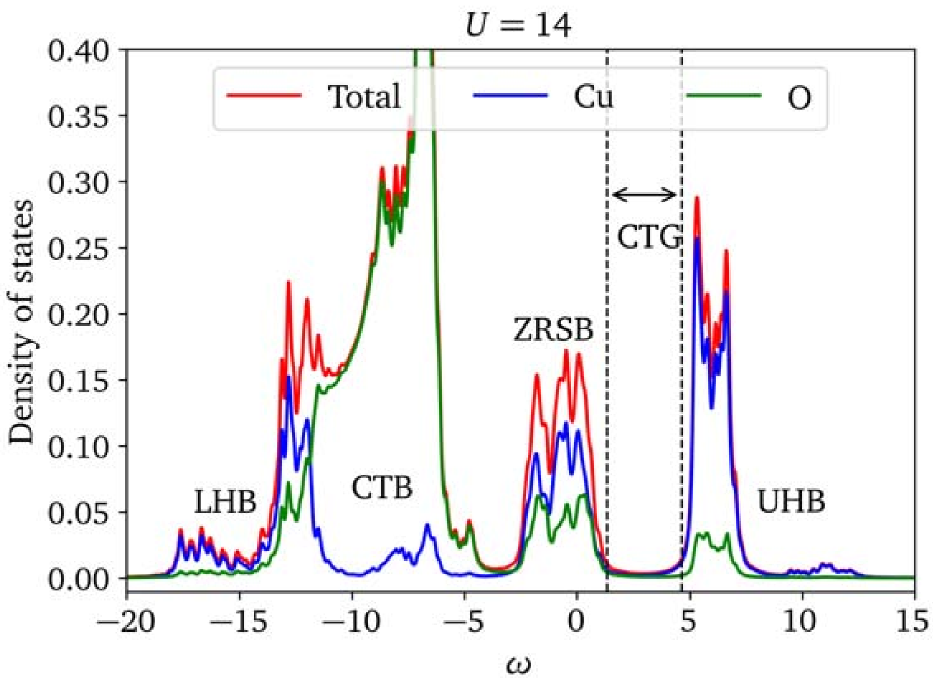
Reduced wave vector

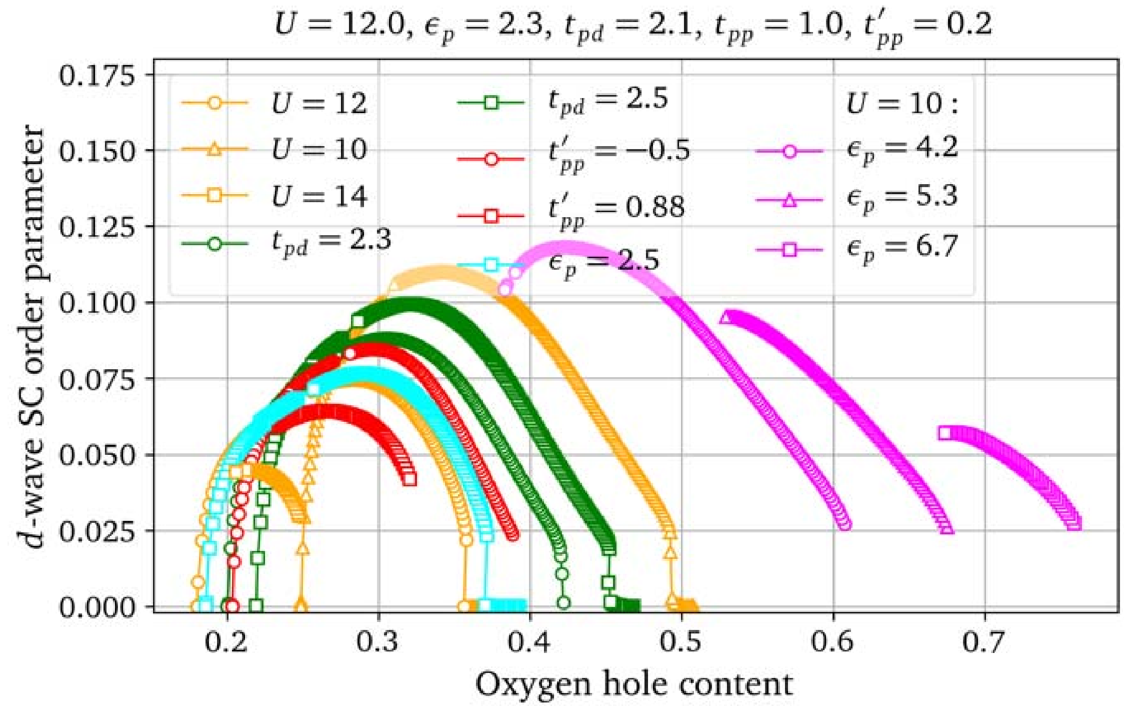
$$\langle\hat{\Delta}\rangle = \oint \frac{d\omega}{2\pi} \frac{d^2\tilde{\mathbf{k}}}{(2\pi)^2}\, tr\left[\mathbf{\Delta}(\tilde{\mathbf{k}})\mathbf{G}(\tilde{\mathbf{k}}, \omega)\right]$$

Average per site

Green function from CDMFT

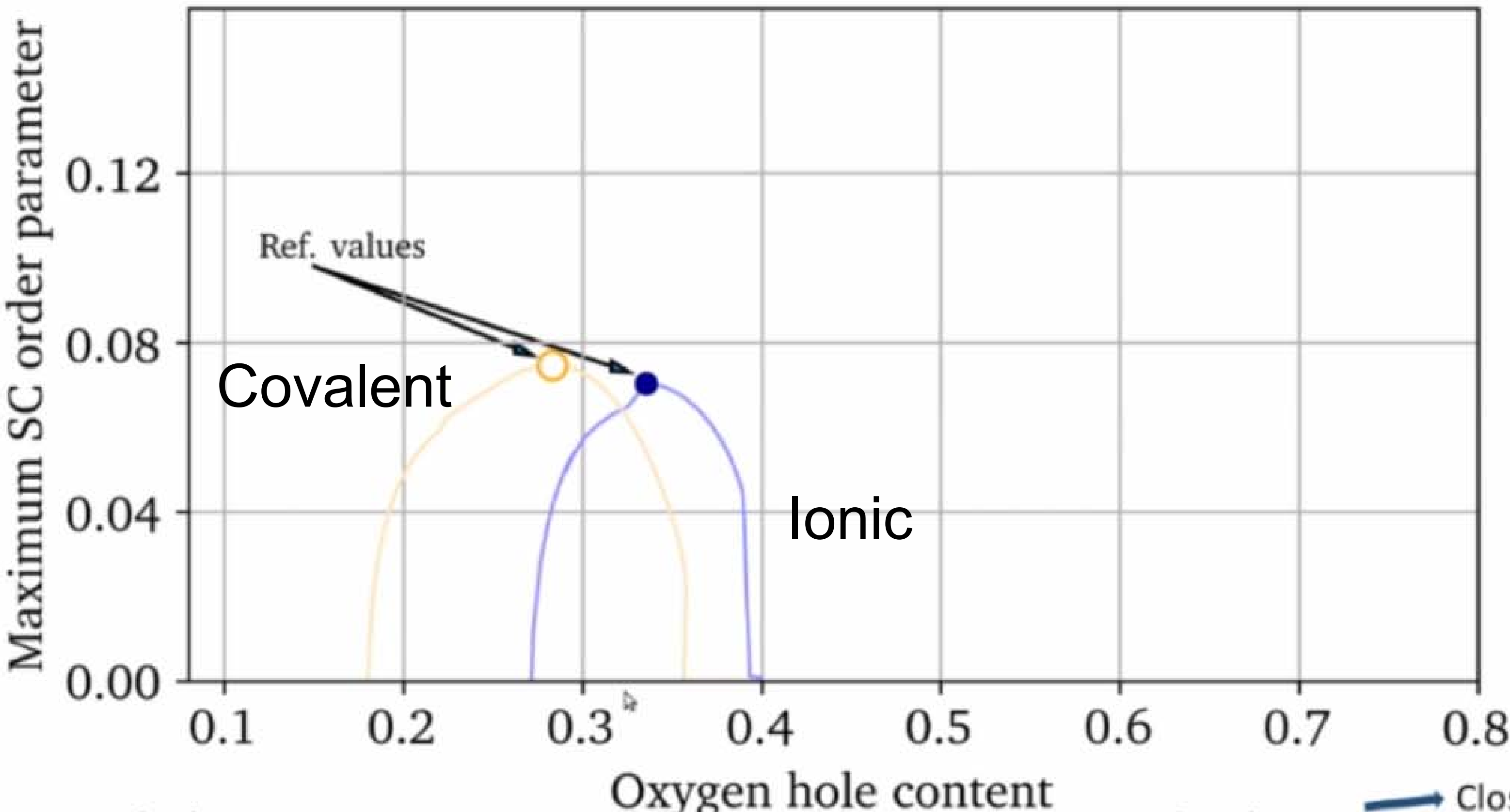
$T = 0$ superconducting domes for the covalent models





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

$T = 0$ superconducting domes for the reference models



Ionic case

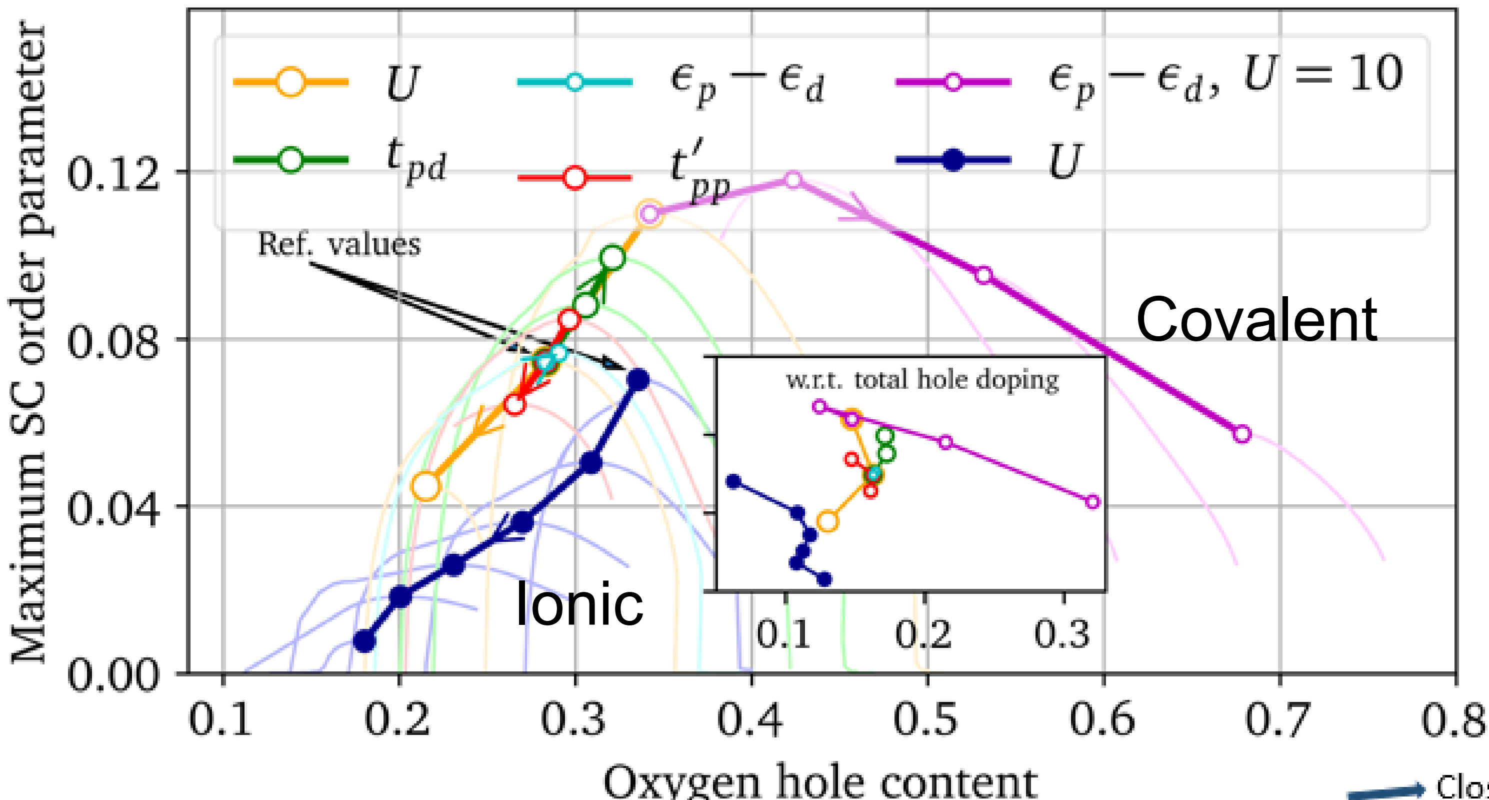
Closer to cuprates

Covalent case

● $U = 12$, $\epsilon_p - \epsilon_d = 7.0$, $t_{pd} = 1.5$, $t_{pp} = 1.0$, $t'_{pp} = 1.0$ ○ $U = 12$, $\epsilon_p - \epsilon_d = 2.3$, $t_{pd} = 2.1$, $t_{pp} = 1.0$, $t'_{pp} = 0.2$

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

T = *0* max order parameter for the two models



Closer to cuprates

Ionic case

Covalent case

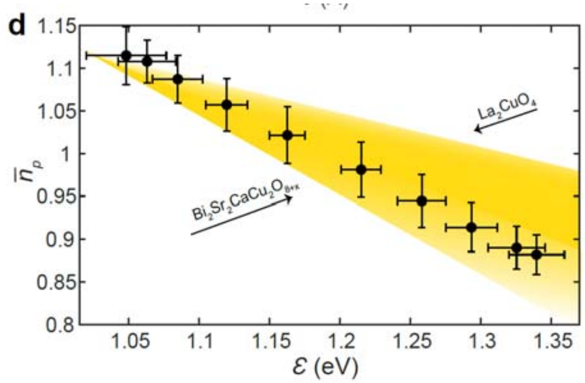
● $U = 12, \epsilon_p - \epsilon_d = 7.0, t_{pd} = 1.5, t_{pp} = 1.0, t'_{pp} = 1.0$ ○ $U = 12, \epsilon_p - \epsilon_d = 2.3, t_{pd} = 2.1, t_{pp} = 1.0, t'_{pp} = 0.2$

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

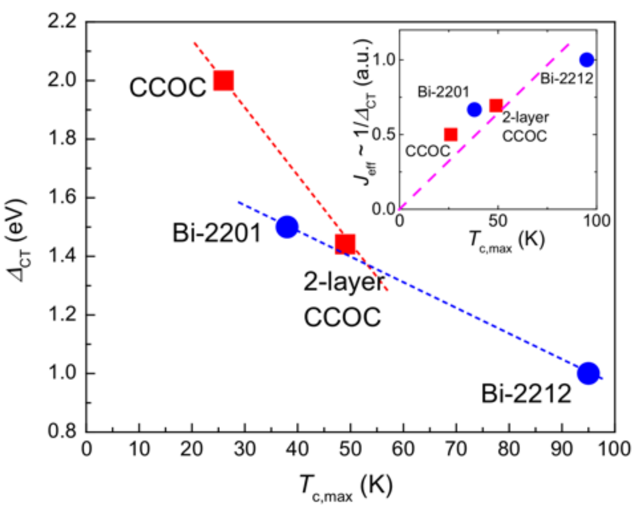
#2 Optimizing T_c with Charge Transfer gap ϵ

(Oxygen as a witness)

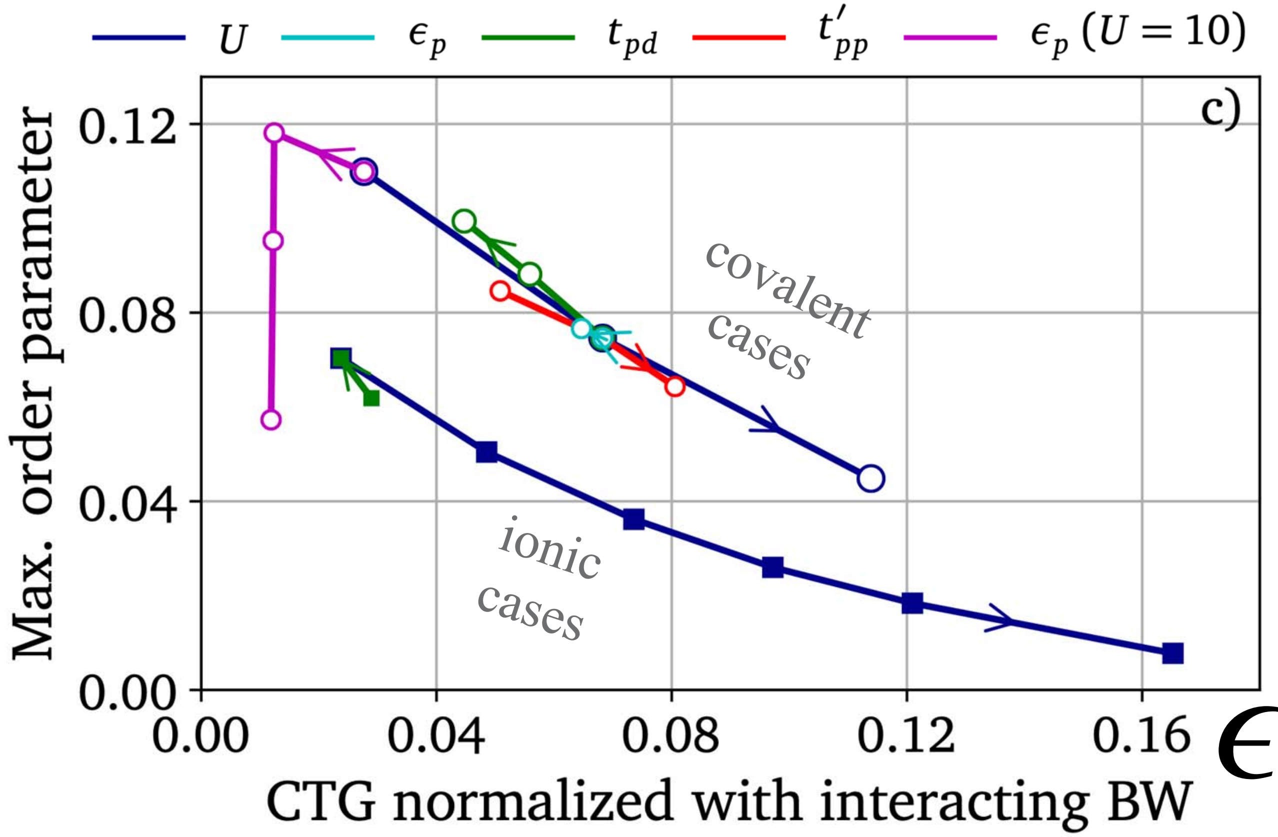
#2 Optimizing T_c with CT gap Δ (Oxygen as a witness)



O'Mahony *et al.* arXiv:2108.03655

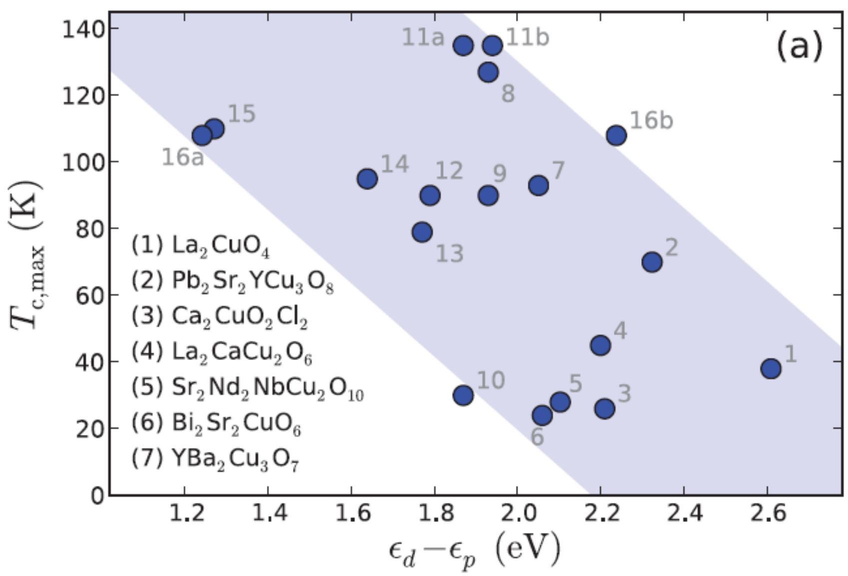


Ruan *et al.* Sci. Bull. **61** (2016)

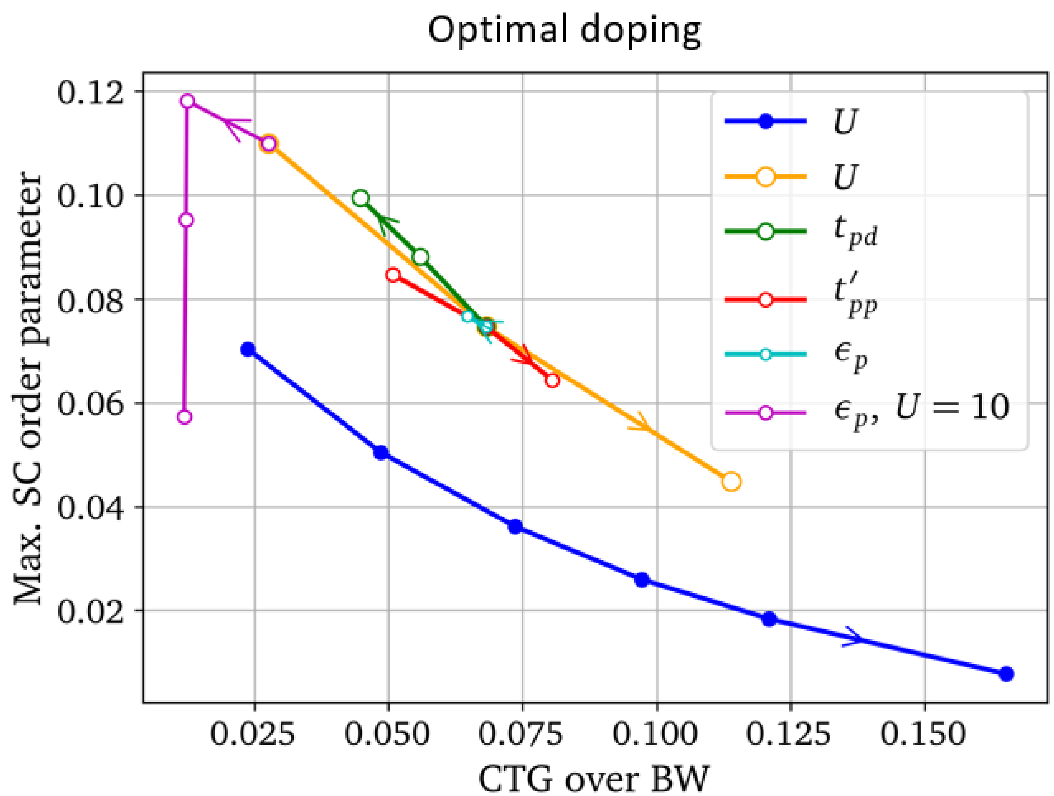


Kowalski, Dash, Sémon, Sénéchal, A-M.T.
PNAS **118** (40) e2106476118 (2021)

Experimental puzzle #2 with Charge Transfer Gap



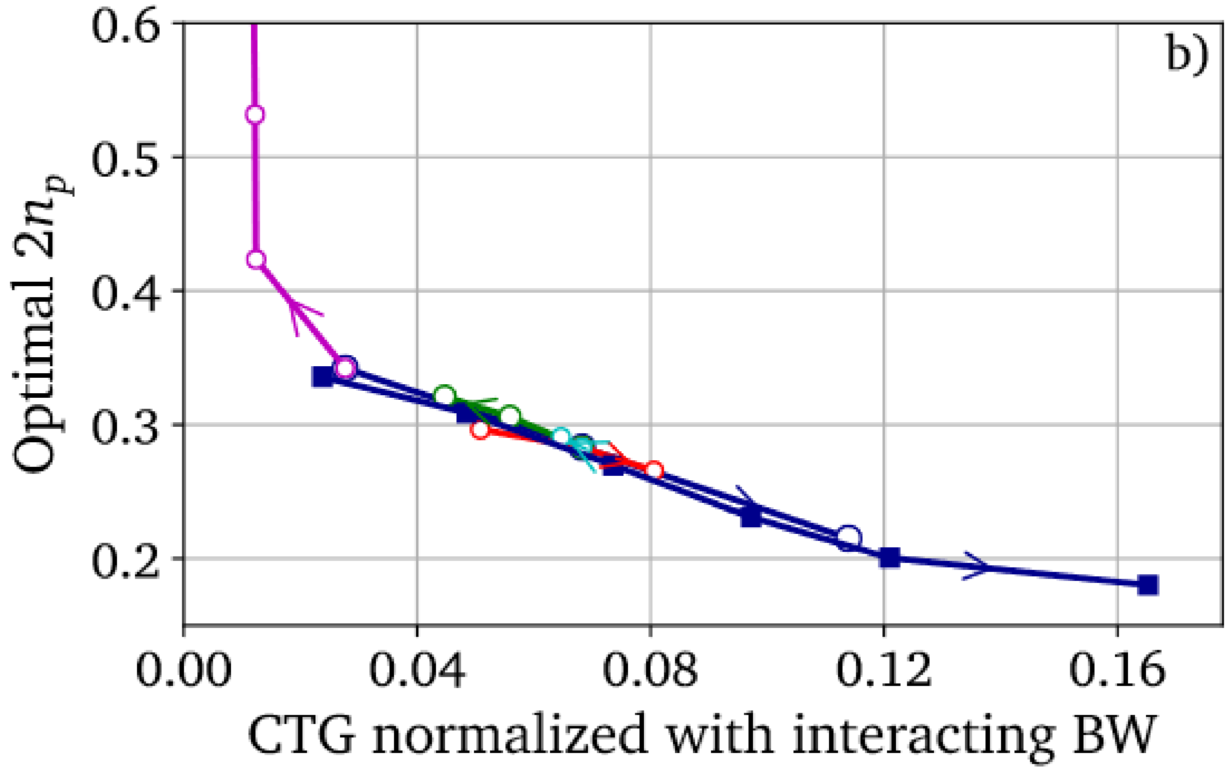
Weber, Yee, Haule, Kotliar, EPL 100, 2012



Acharya et al. Phys. Rev. X 8, 021038 (2018)

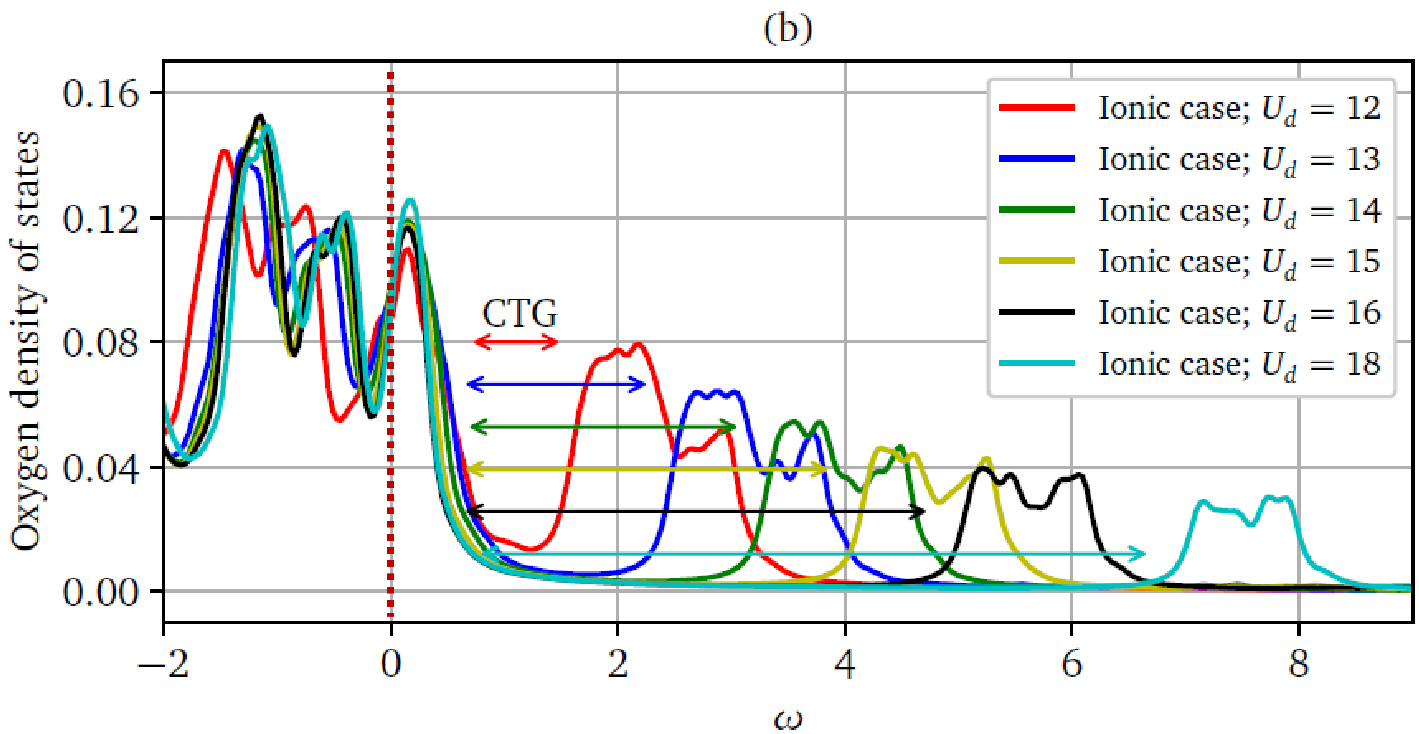
Kowalski, Dash, Sémon, Sénéchal, A-M.T.
PNAS **118** (40) e2106476118 (2021)

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

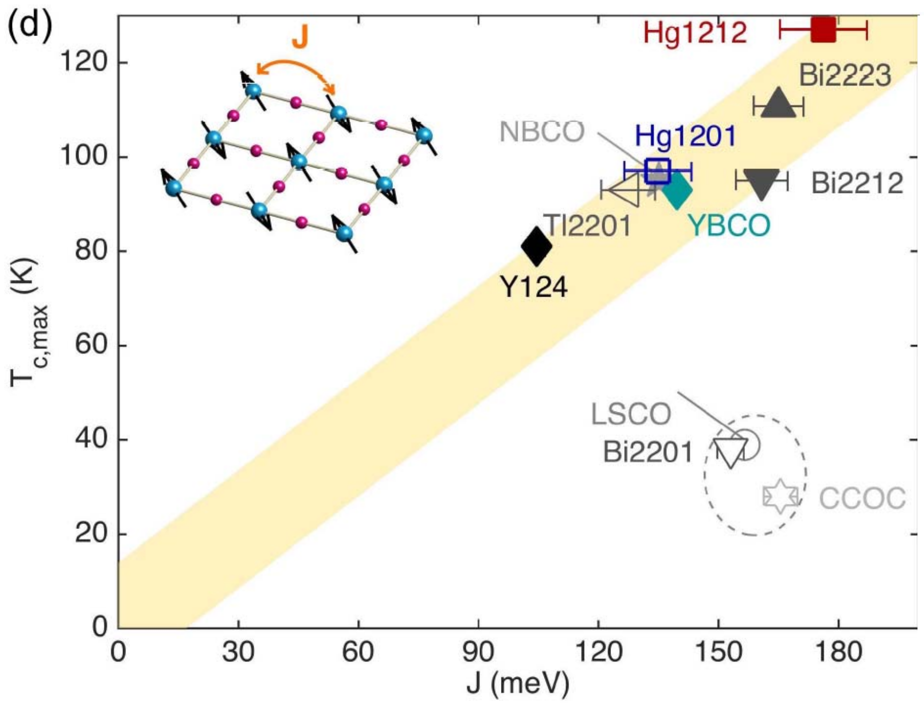


#3 Optimizing T_c with superexchange

#3 Optimizing T_c with superexchange

E. Müller-Hartmann *et al*. Eur. Phys. J. B **28**, 173 (2002)

$$J = \frac{4t_{pd}^4(U+\epsilon)}{U\epsilon^3} \underset{U\to\infty}{\rightarrow} \frac{4t_{pd}^4}{\epsilon^3}$$



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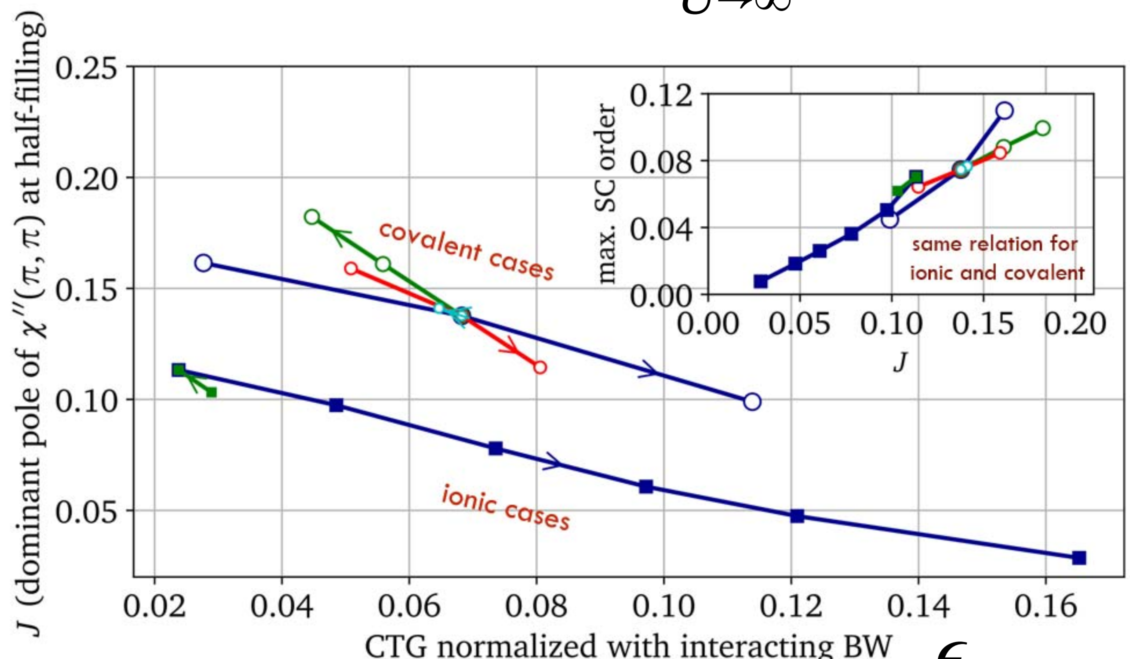

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Super exchange

E. Müller-Hartmann *et al.* Eur. Phys. J. B **28**, 173 (2002)

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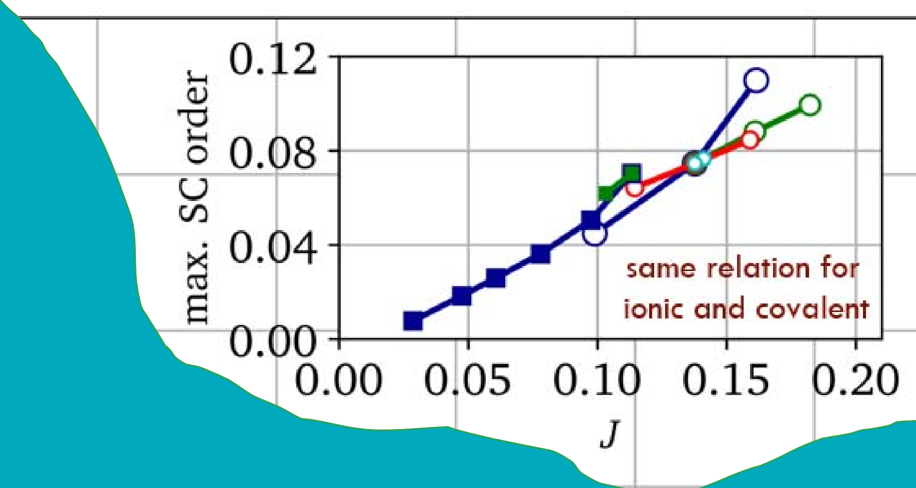

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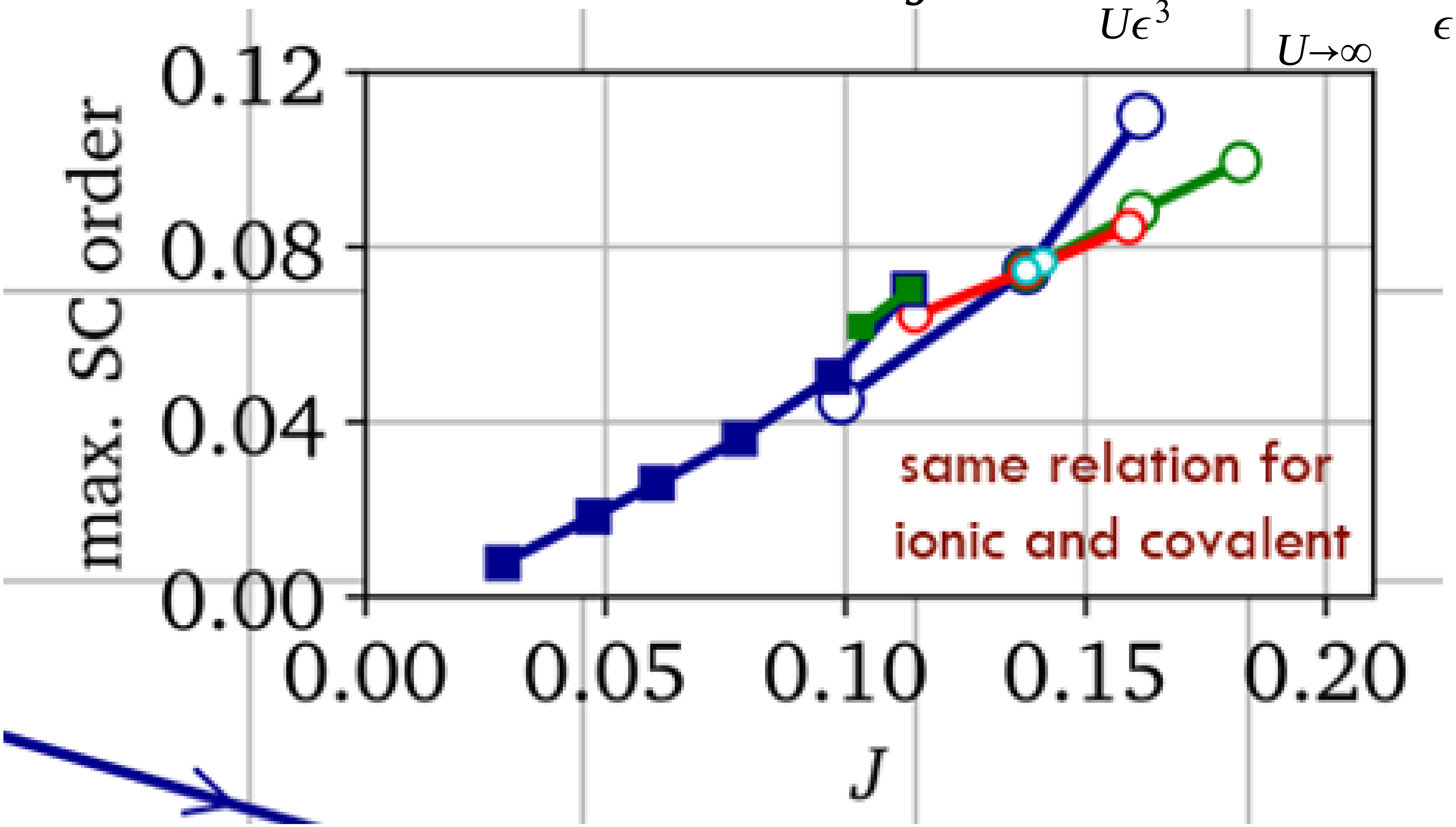

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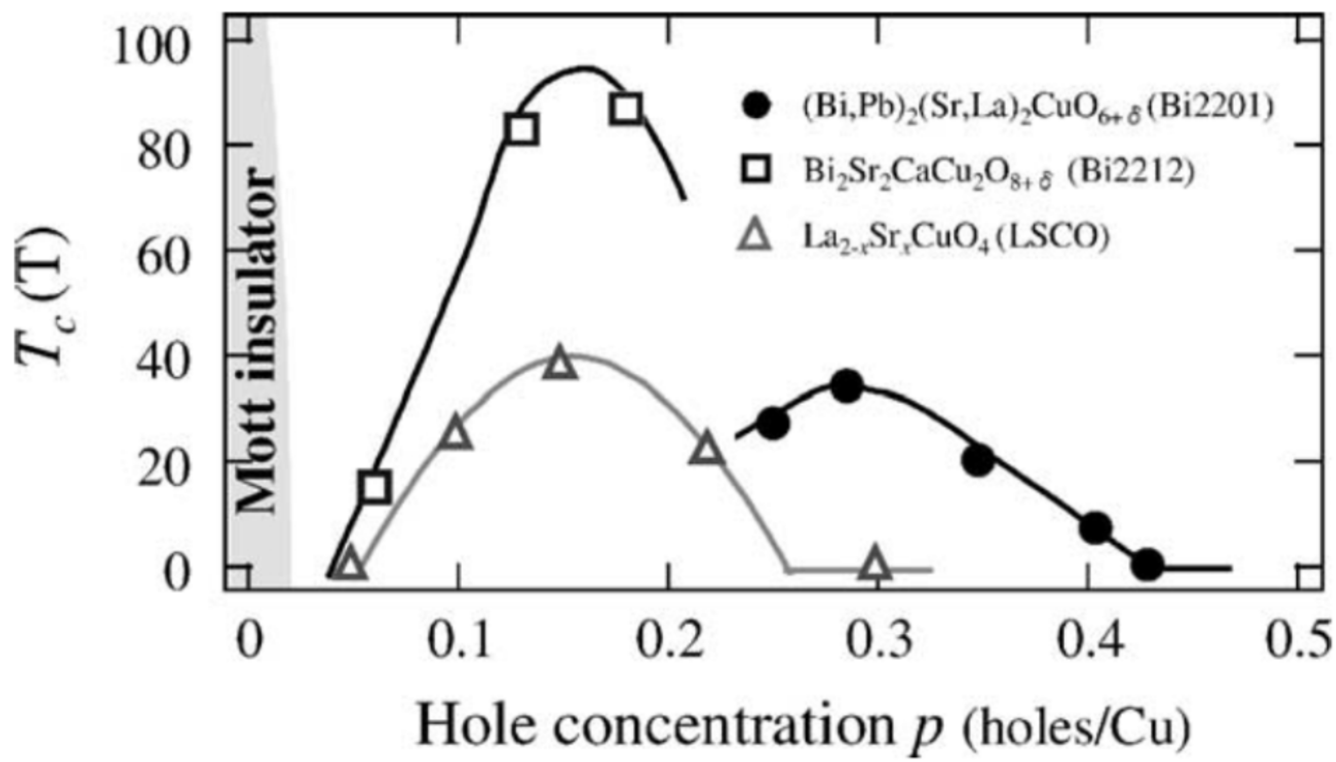
Bonus

T_c and total hole concentration are not well correlated



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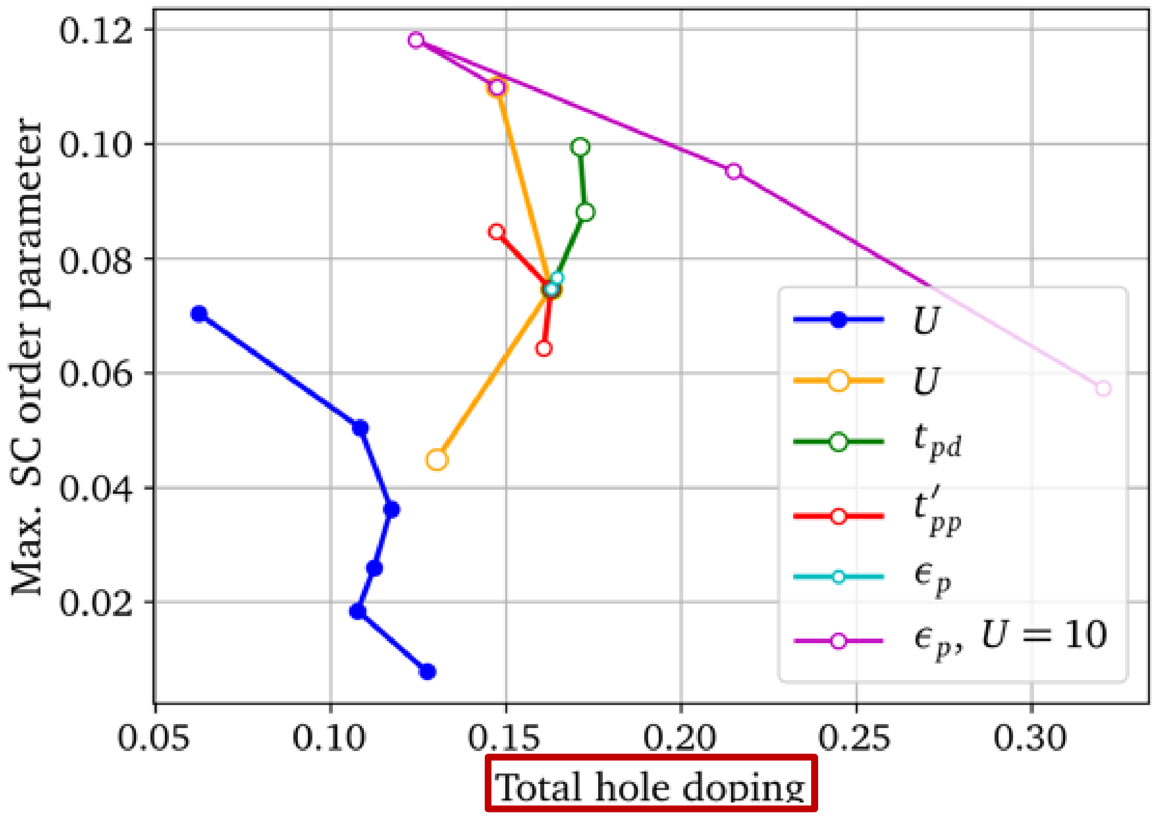
Journal of Electron Spectroscopy and Related Phenomena **137-140**, 663 (2004)

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

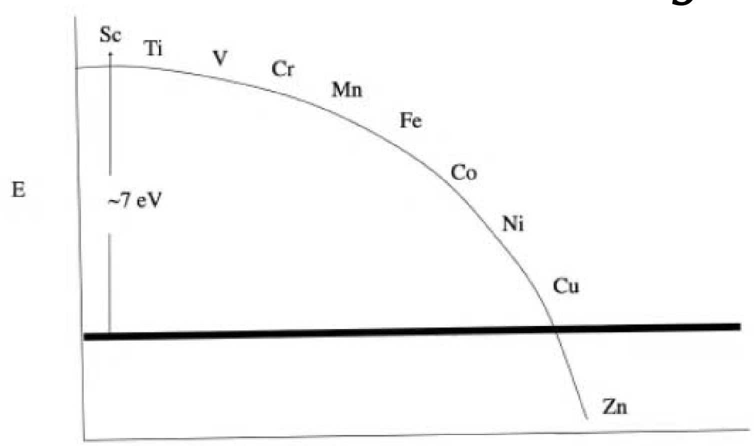


Kowalski, Dash, Sémon, Sénéchal, A-M.T.
PNAS **118** (40) e2106476118 (2021)

Bonus : Importance of covalency

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

$$J = \frac{4t_{pd}^4(U+\epsilon)}{U\epsilon^3} \underset{U\to\infty}{\to} \frac{4t_{pd}^4}{\epsilon^3}$$



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

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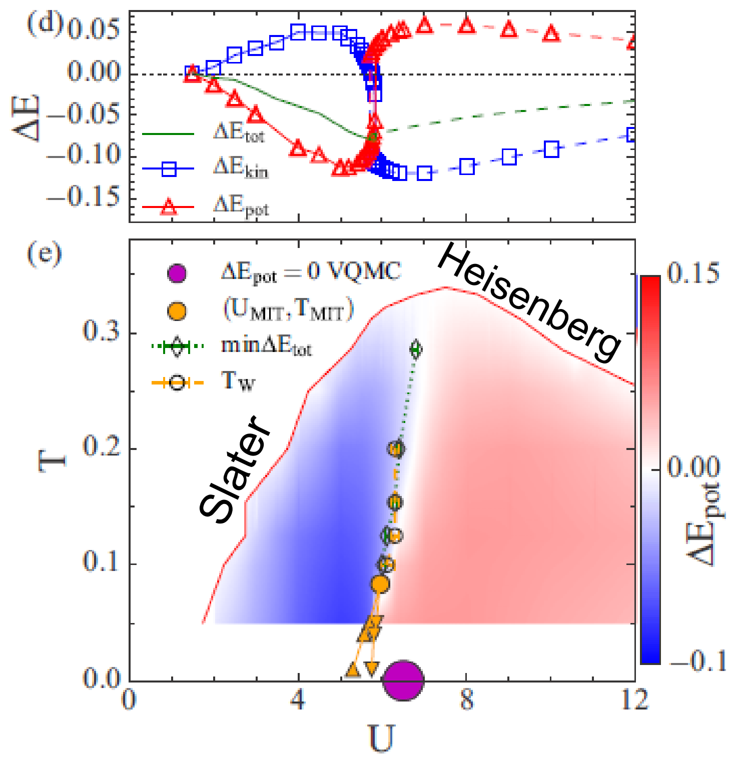
Summary Conclusion

Université de Sherbrooke

Pairing at small and large *U* : An analogy



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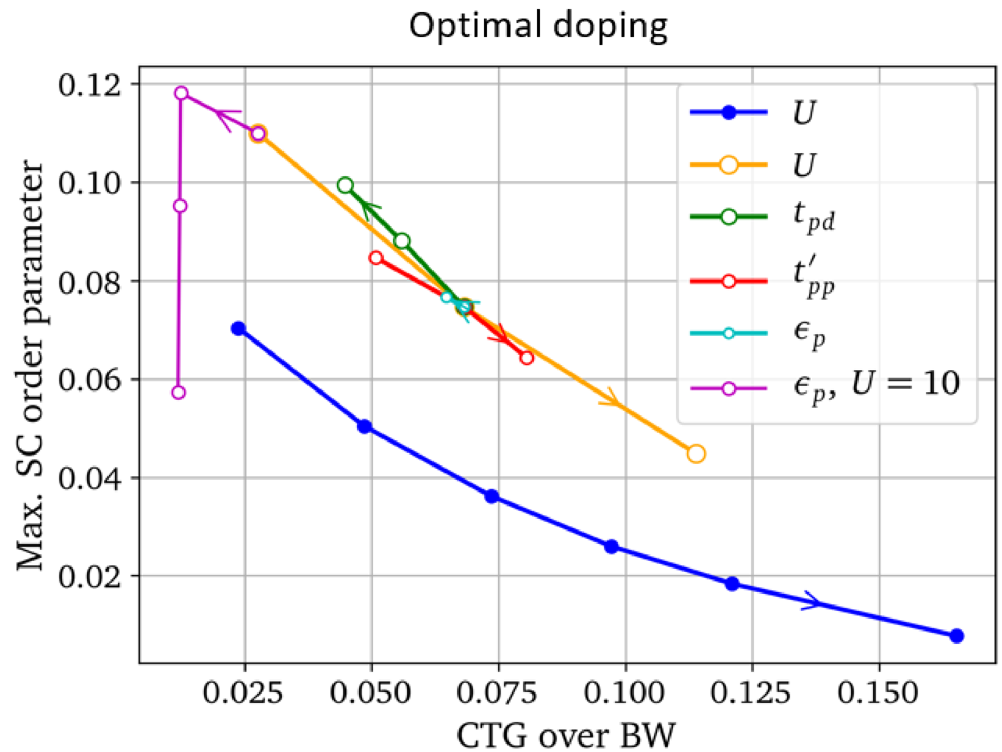

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Weber et al Europhys. Lett. 100, 37001 (2012)
Yee et al Phys. Rev. B 89, 094517 (2014)
Acharya et al Phys. Rev. X 8, 021038 (2018)

Optimizing T*c*

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

C. Weber, PNAS 2021 Vol. **118** No. 46 e2115874118

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

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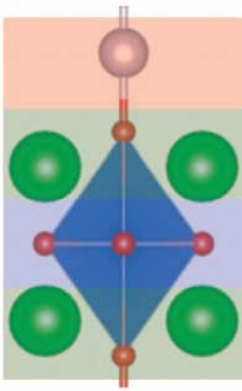
Optimizing T_c



	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)	

$$\mathrm{Hg(CaS)_2CuO_2}$$

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

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.

Merci
Thank you

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