FROM TRANSITION METAL PNICTIDES TO HIGH-THROUGHPUT COMPUTATIONAL SCREENING

61st anniversary of the Centre de Physique Théorique - 24/03/2019

Ambroise van Roekeghem

CPHT Centre de Physique Théorique

A PHD STUDENT IN CPHT : 2011-2014

61st anniversary of the Centre de Physique Théorique - 24/03/2019

Ambroise van Roekeghem

HAVING 2 ADVISORS, A GOOD IDEA ?

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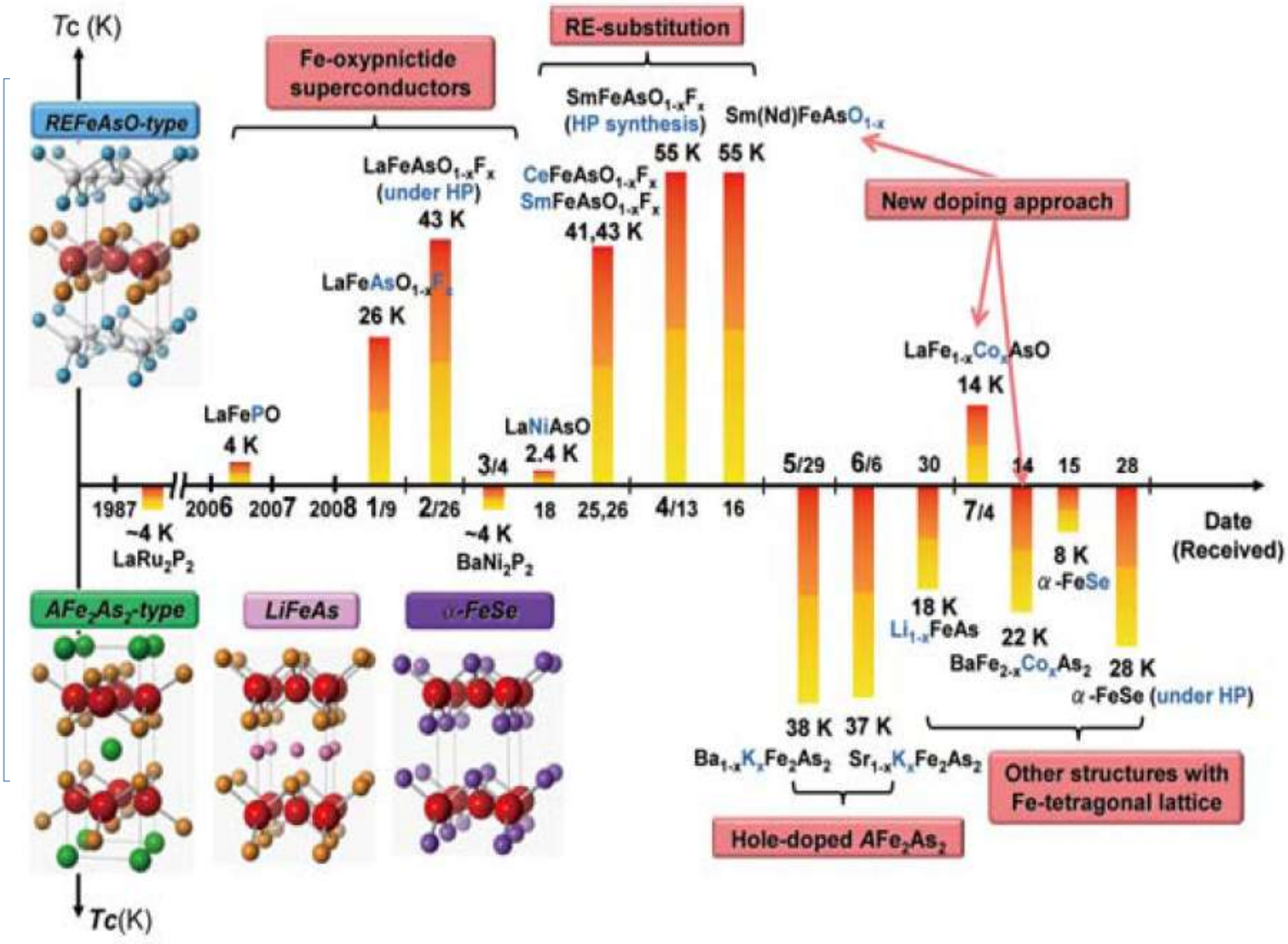
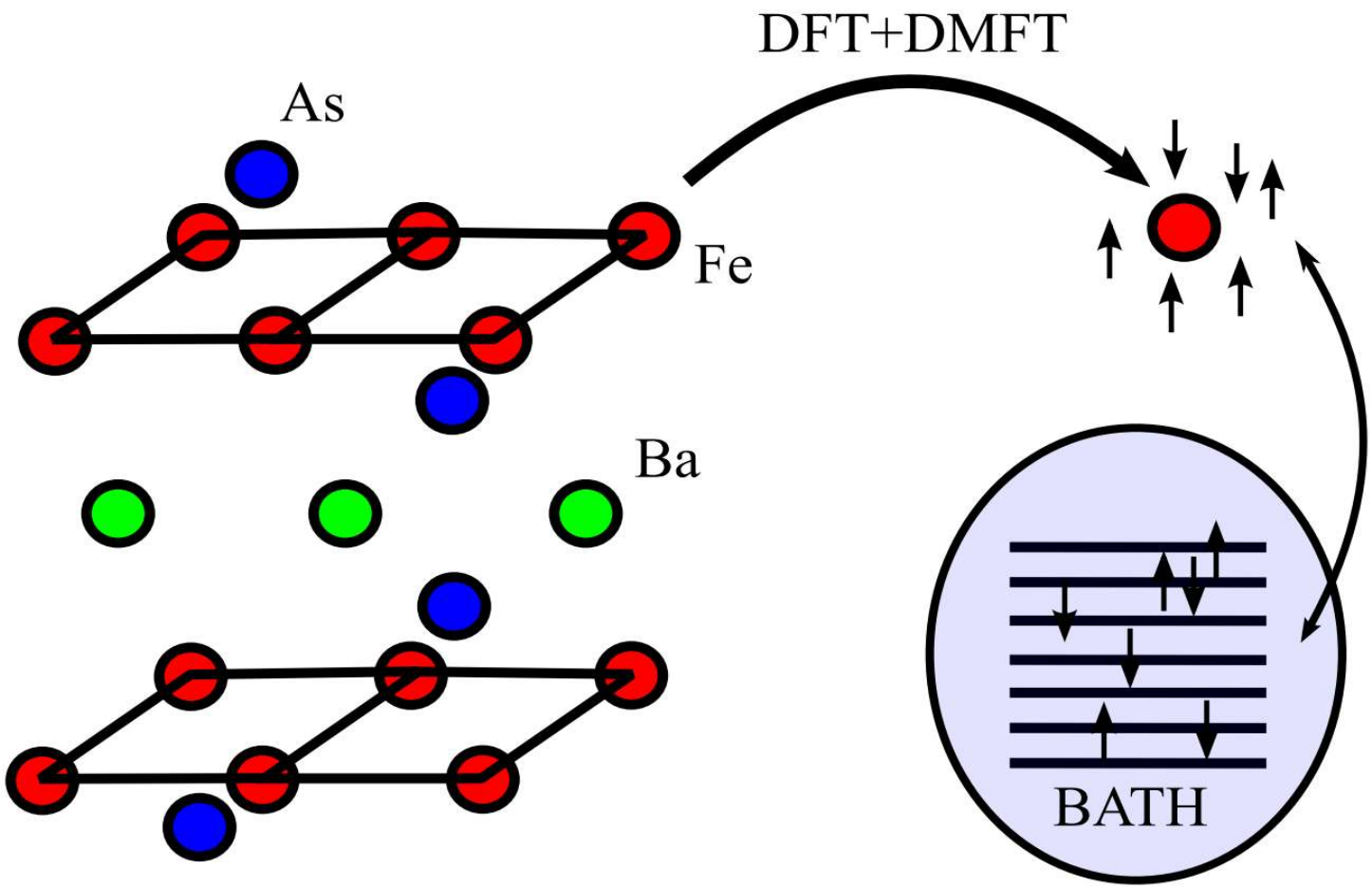
SUPERCONDUCTIVITY IN IRON PNICTIDES



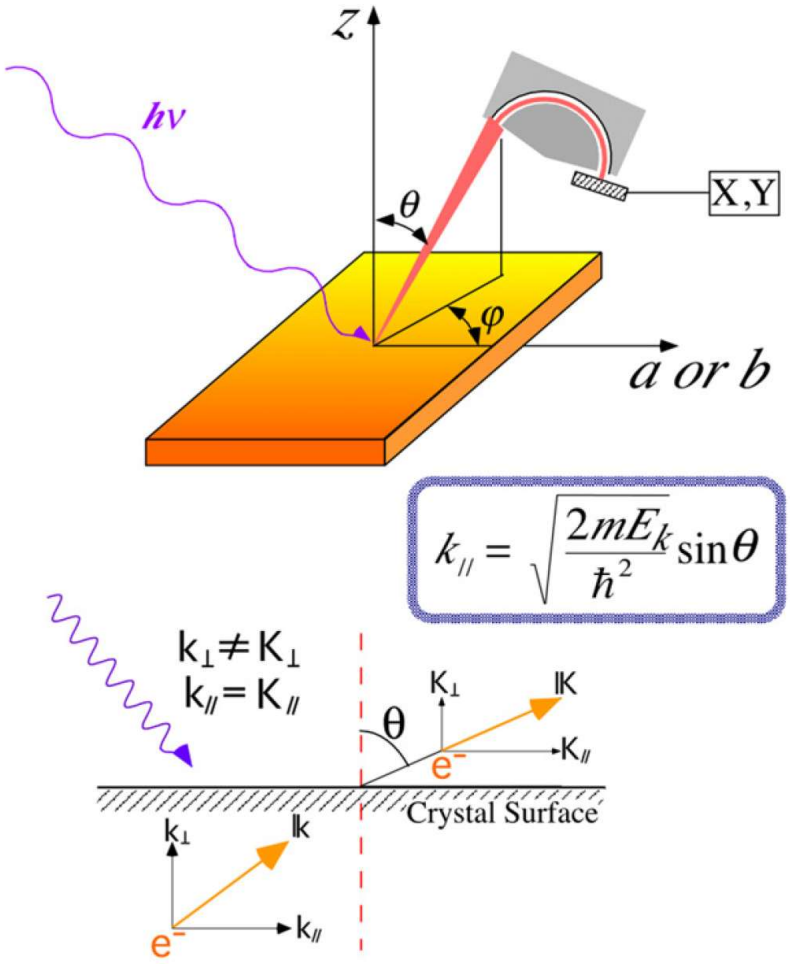
Hosono, J. Phys. Soc. Jpn. 77 (2008)(Suppl. C): 1

THEORY...



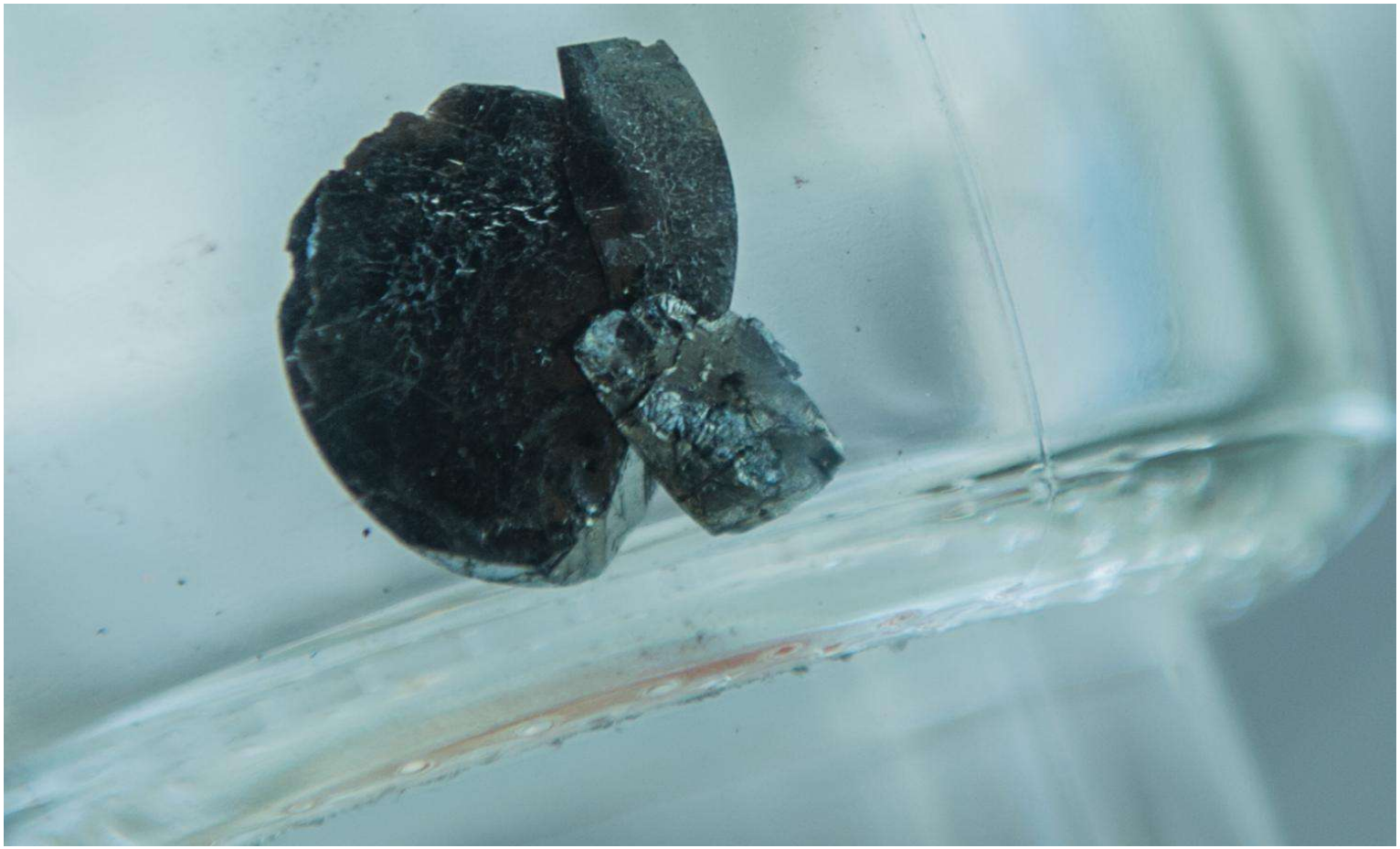
van Roekeghem, Richard, Ding and Biermann, C.R. Phys. 17 (1), 140–163 (2016)

...AND EXPERIMENT



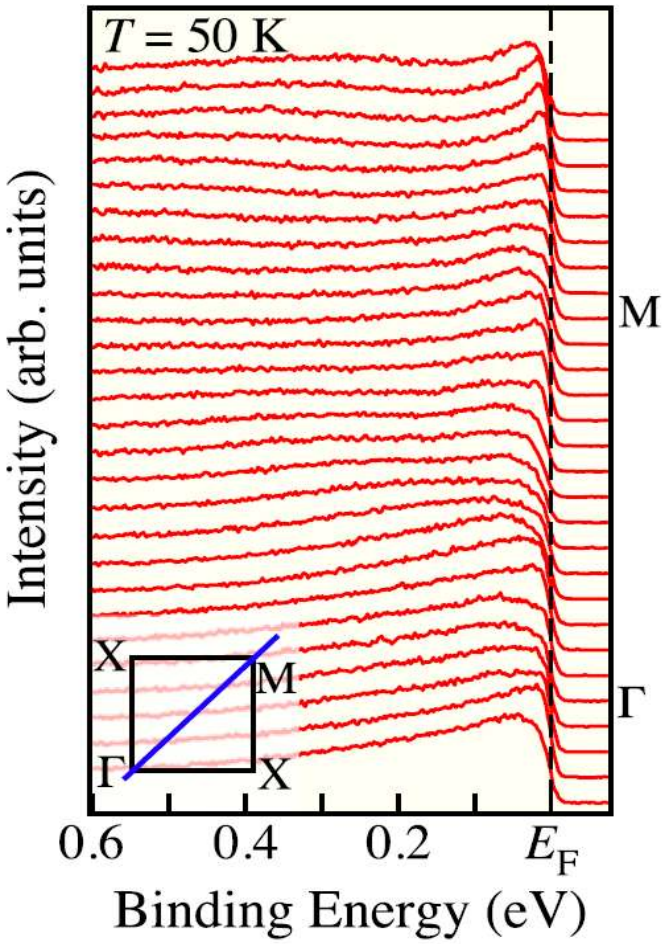
Richard *et al*, Rep. Prog. Phys. 74 (2011): 124512

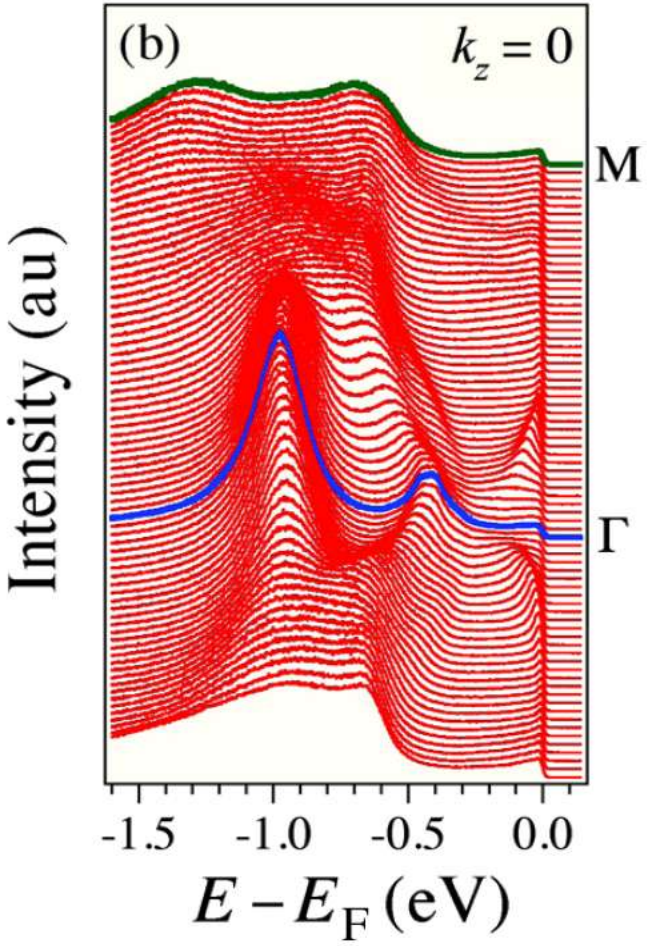
DOES IT LOOK GOOD ?



Credit: Jeff Fitlow/Rice University

FROM BA0.6K0.4FE2AS2 TO BACO2AS2

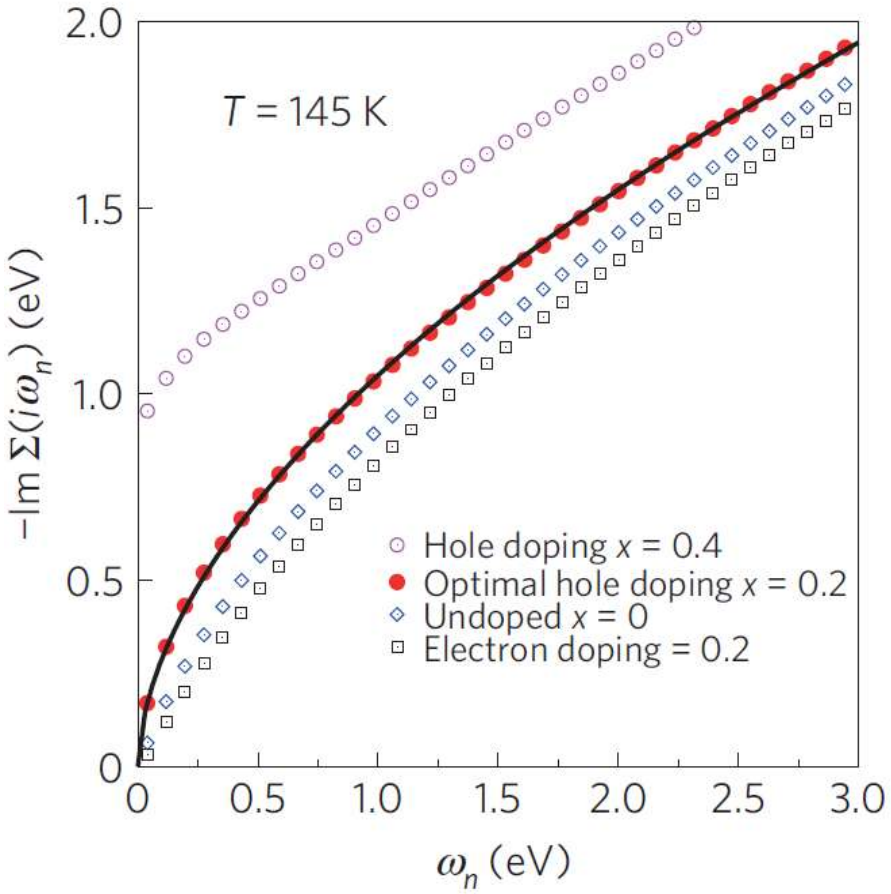


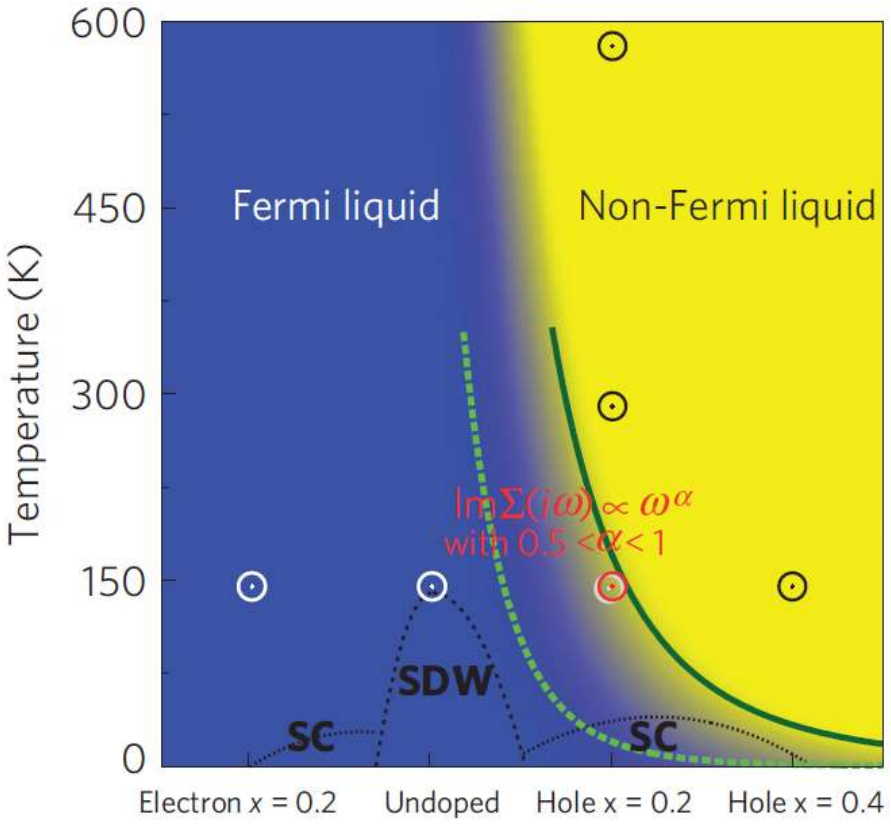


Ding *et al*, J. Phys.: Cond. Matt. 23 (2011) 135701

Xu *et al*, Phys. Rev. X 3 (2013): 011006

DOPING BAFE2AS2





Werner *et al*, Nature Physics 8 (2012): 331


Bât. Paul LEVY

THEORETICIANS DOING EXPERIMENTS

EXPECTED THINGS

UNEXPECTED THINGS

Having 2 advisors, a good idea?

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Having 2 advisors, a good idea?

PRL 119, 056401 (2017) PHYSICAL REVIEW LETTERS week ending 4 AUGUST 2017

Towards a First-Principles Determination of Effective Coulomb Interactions in Correlated Electron Materials: Role of Intershell Interactions

Priyanka Seth,[1] Philipp Hansmann,[1,2] Ambroise van Roekeghem,[1,3] Loig Vaugier,[1] and Silke Biermann[1]
[1]*Centre de Physique Théorique, Ecole Polytechnique, CNRS, Université Paris-Saclay, 91128 Palaiseau, France*
[2]*Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany*
[3]*Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*
(Received 21 August 2015; revised manuscript received 22 July 2016; published 4 August 2017)

epl A Letters Journal Exploring the Frontiers of Physics September 2012
EPL, **99** (2012) 67001 www.epljournal.org
doi: 10.1209/0295-5075/99/67001

Observation of an isotropic superconducting gap at the Brillouin zone centre of $Tl_{0.63}K_{0.37}Fe_{1.78}Se_2$

X.-P. Wang[1,2], P. Richard[1(a)], X. Shi[1], A. Roekeghem[1,3], Y.-B. Huang[1], E. Razzoli[2], T. Qian[1], E. Rienks[4], S. Thirupathaiah[4], H.-D. Wang[5], C.-H. Dong[5], M.-H. Fang[5], M. Shi[2] and H. Ding[1(b)]

received on 27 August 2012; accepted by J. Fink on 27 August 2012
published online 12 September 2012

Having 2 advisors, a good idea?

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PHYSICAL REVIEW X **3**, 011006 (2013)

Electronic Band Structure of $BaCo_2As_2$: A Fully Doped Ferropnictide Analog with Reduced Electronic Correlations

N. Xu,[1] P. Richard,[1,*] A. van Roekeghem,[1,2] P. Zhang,[1] H. Miao,[1] W.-L. Zhang,[1]
T. Qian,[1] M. Ferrero,[2] A. S. Sefat,[3] S. Biermann,[2,4] and H. Ding[1]

[1]*Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*

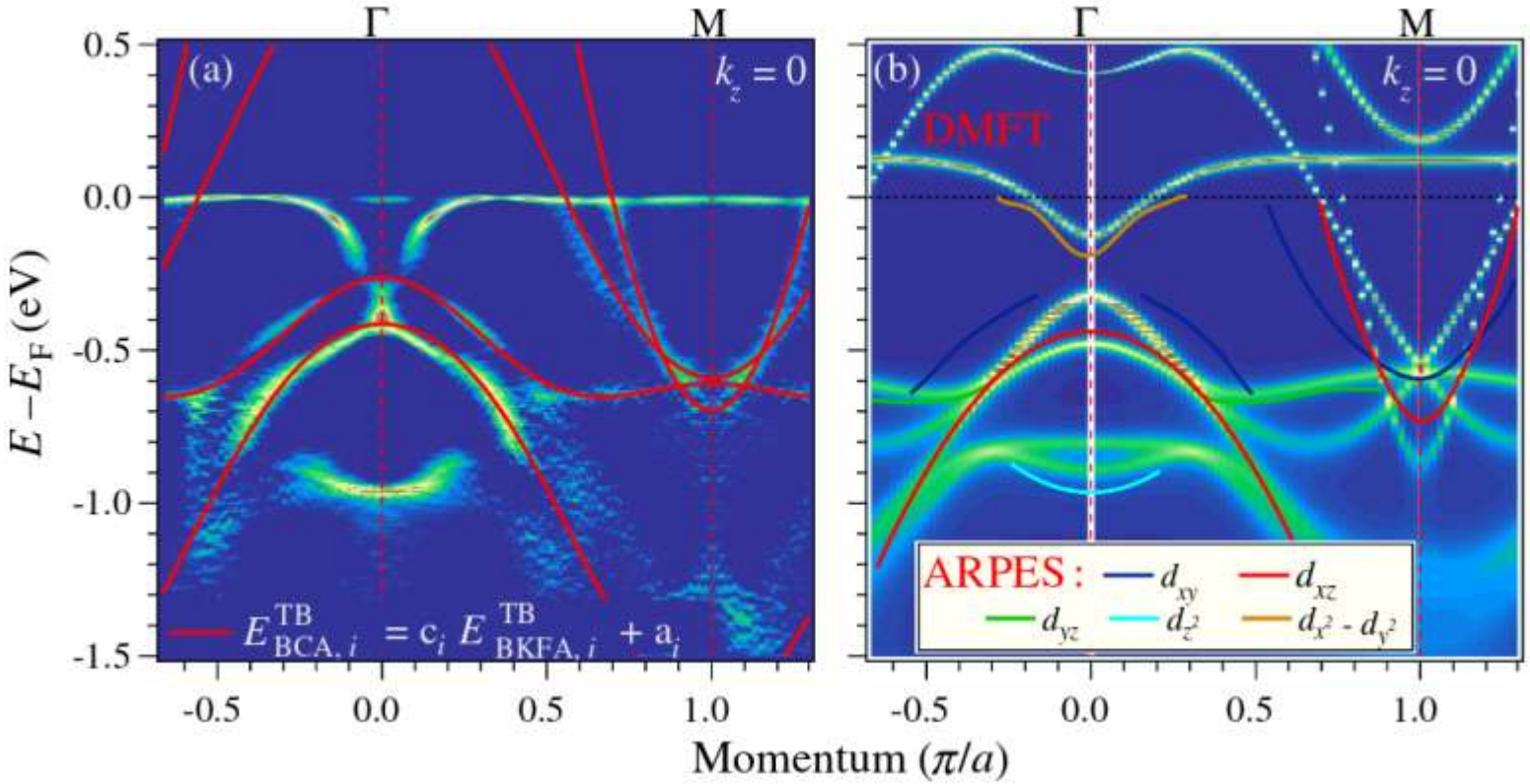
[2]*Centre de Physique Théorique, Ecole Polytechnique, CNRS-UMR7644, 91128 Palaiseau, France*

[3]*Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831-6114, USA*

[4]*Japan Science and Technology Agency, CREST, Kawaguchi 332-0012, Japan*

(Received 18 October 2012; published 28 January 2013)

Having 2 advisors, a good idea?



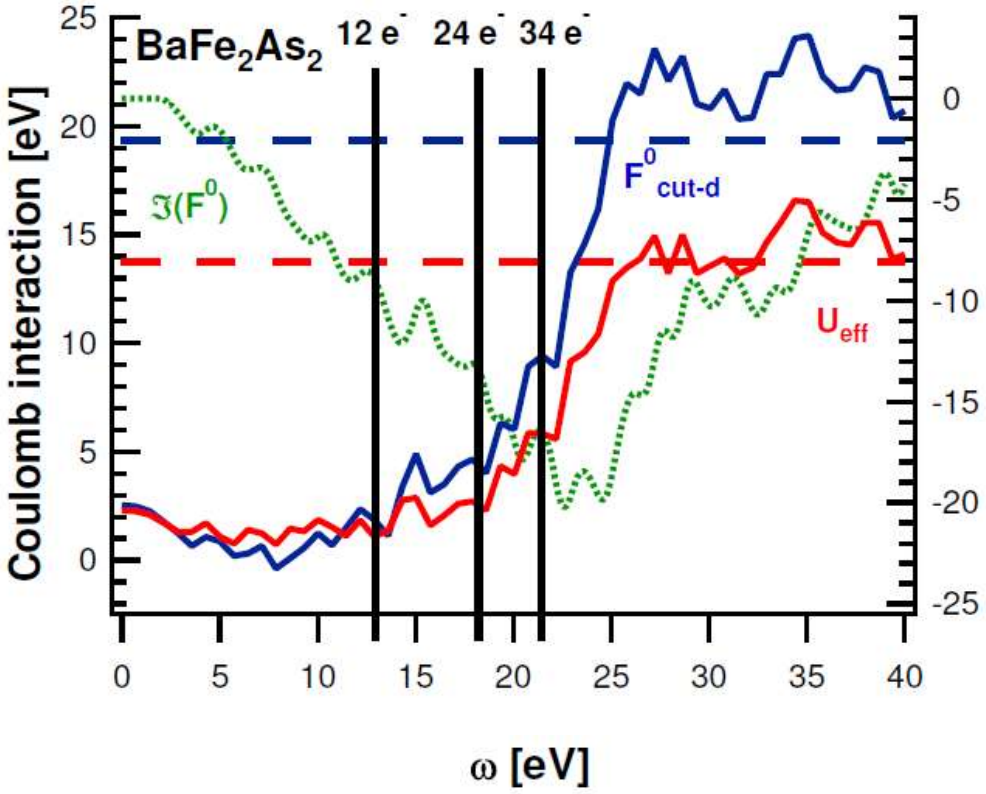
Xu *et al*, Phys. Rev. X 3 (2013): 011006

Screening of Coulomb interaction

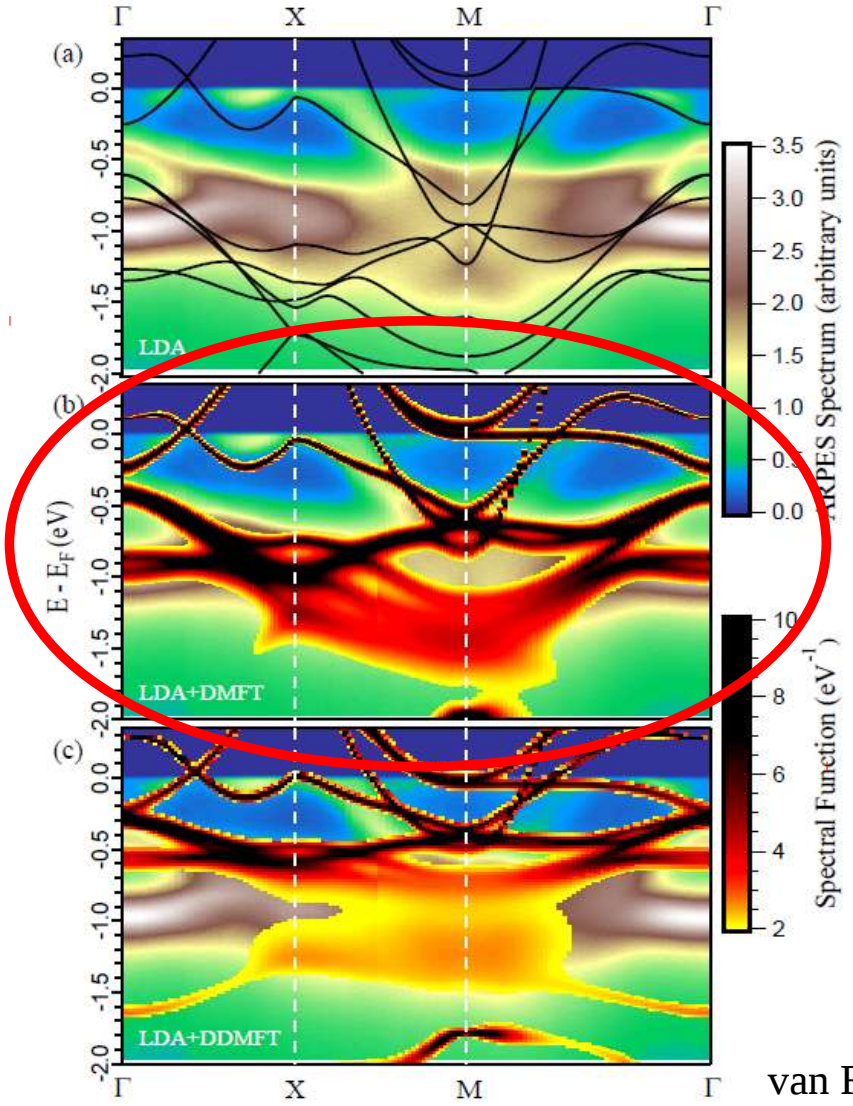
$$H_{loc} = V n_\uparrow n_\downarrow + \lambda(n_\uparrow + n_\downarrow)(b^\dagger + b) + \omega_0 \left(b^\dagger b + \frac{1}{2} \right)$$

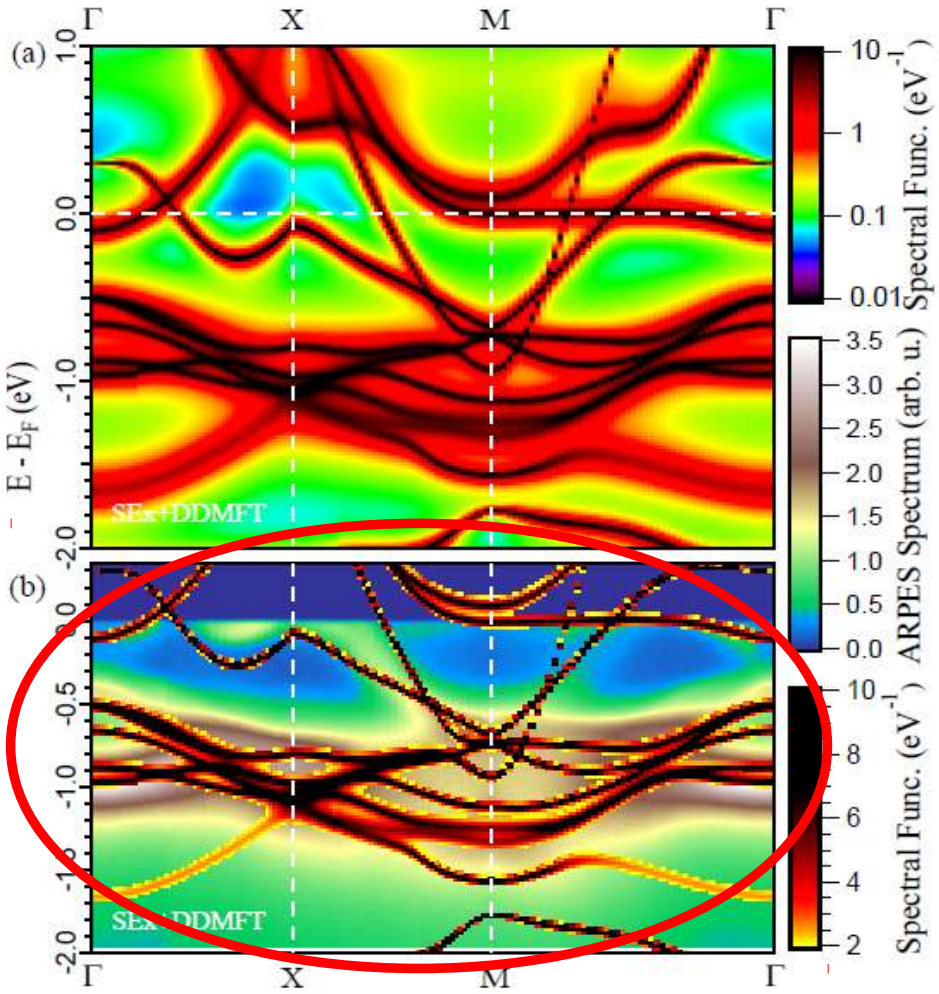
Formation of electronic polarons with enhanced effective mass and screened Coulomb interaction

$$\tilde{H}_{loc} = (V - 2\frac{\lambda^2}{\omega_0})\tilde{n}_\uparrow \tilde{n}_\downarrow - \frac{\lambda^2}{\omega_0}(\tilde{n}_\uparrow + \tilde{n}_\downarrow) + \omega_0 \left(b^\dagger b + \frac{1}{2} \right)$$



The SEX+DDMFT method





van Roekeghem *et al*, Phys. Rev. Lett. 113, 266403 (2014)

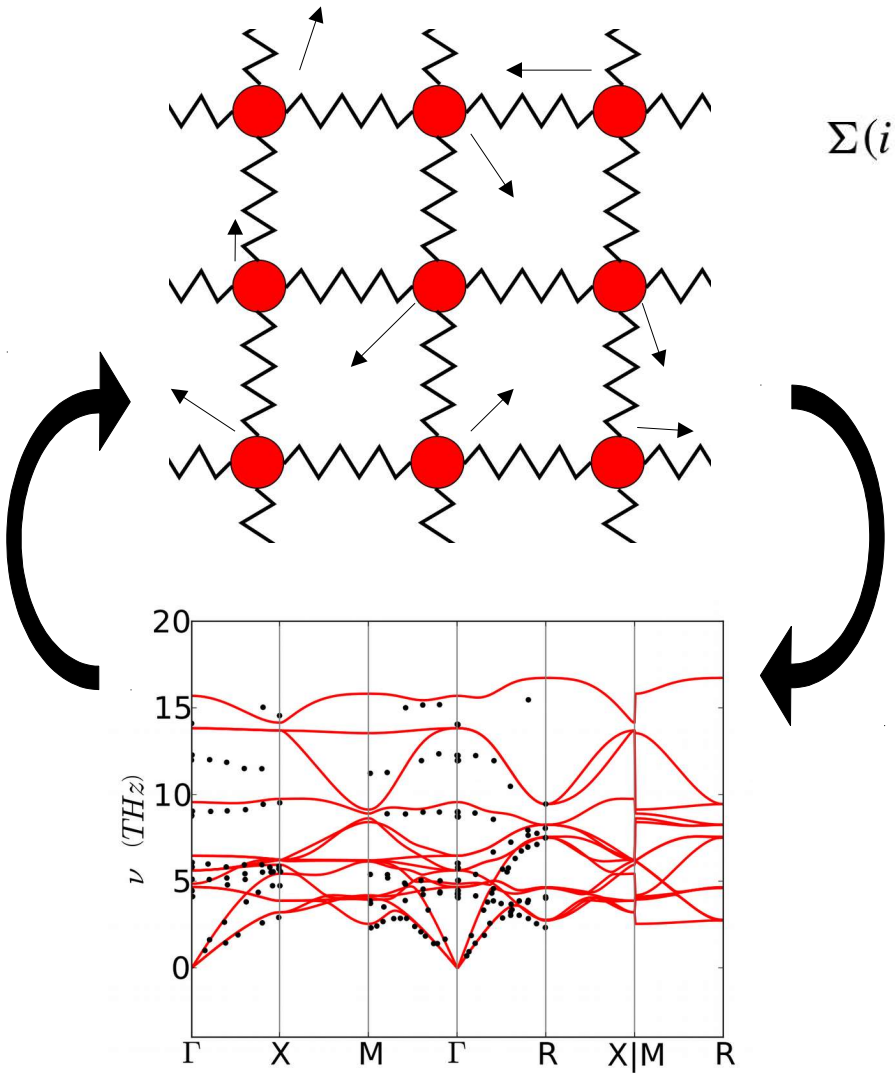
WHERE IS MASSIMO ?

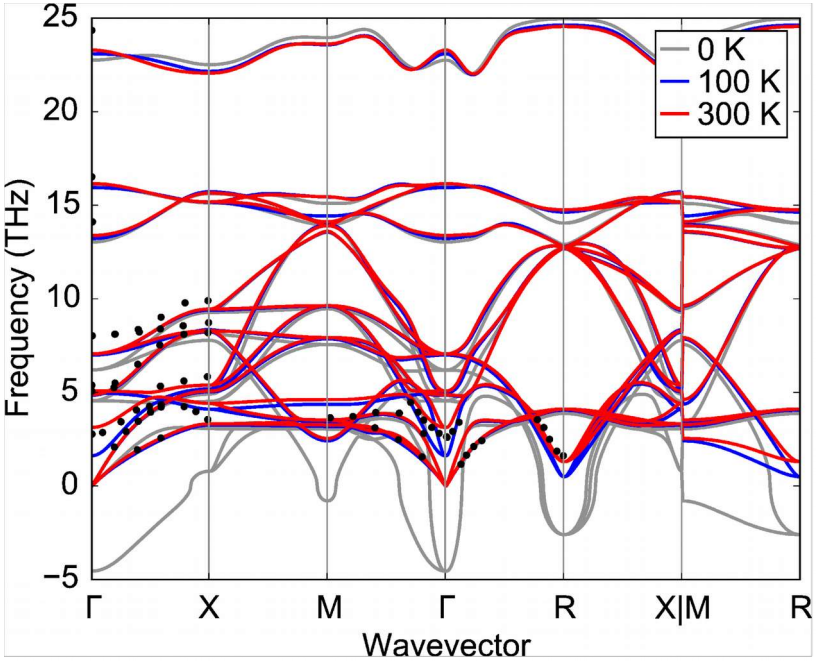
COMPUTING PHONONS

Quantum statistics, finite T

$$\rho_h(\{u_{i\alpha}\}) \propto \exp\left(-\tfrac{1}{2}u^T \Sigma^{-1} u\right)$$

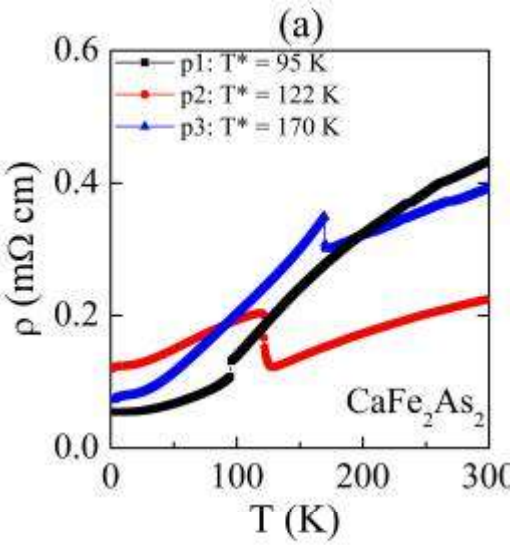
$$\Sigma(i\alpha, j\beta) = \frac{\hbar}{2\sqrt{M_i M_j}} \sum_m \omega_m^{-1}[1 + 2n_B(\omega_m)]\epsilon_{mi\alpha}\epsilon^*_{mj\beta}$$

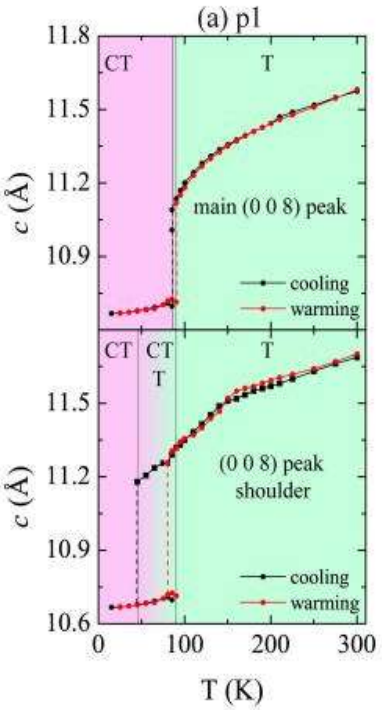




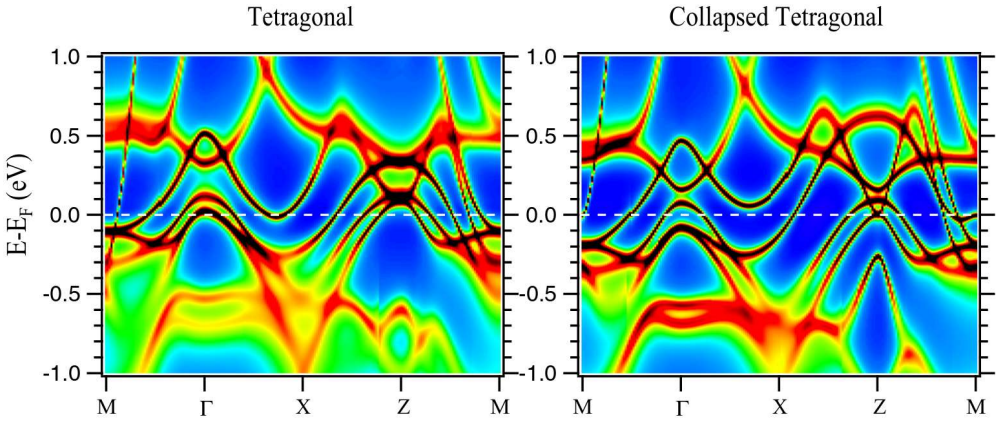
Exp. data at 300 K: Cowley, Phys. Rev. 134, A981 (1964) and Stirling, J. Phys. C: Solid State Physics 5, 2711 (1972)

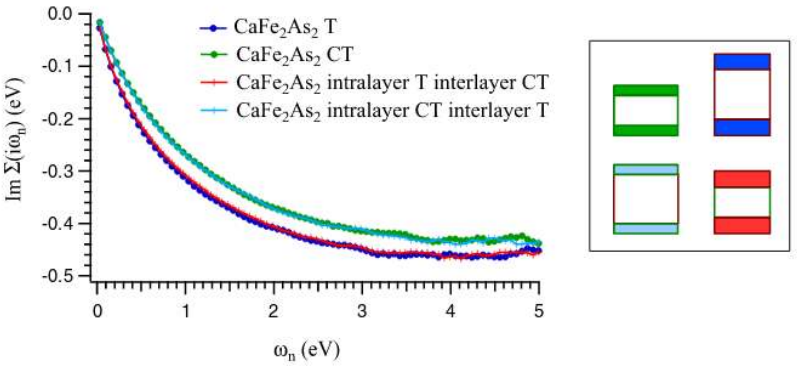
CORRELATIONS OR PHONONS?





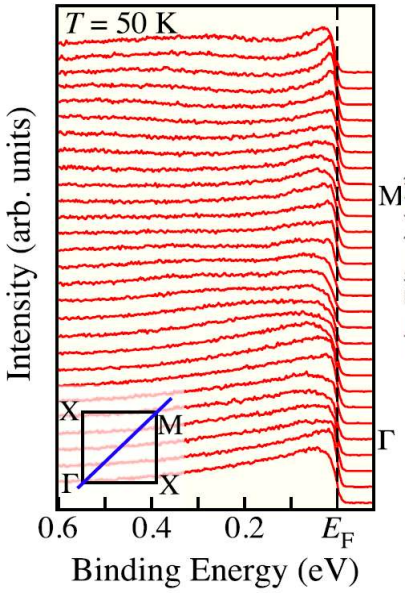
Saparov et al., Sci. Rep. 4, 4120 (2014)

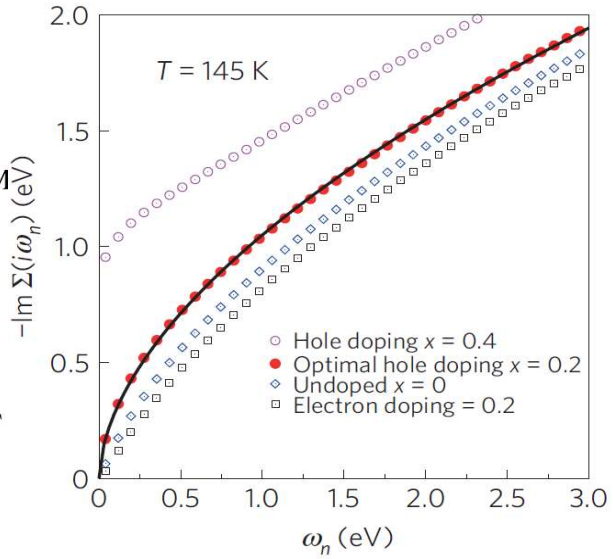


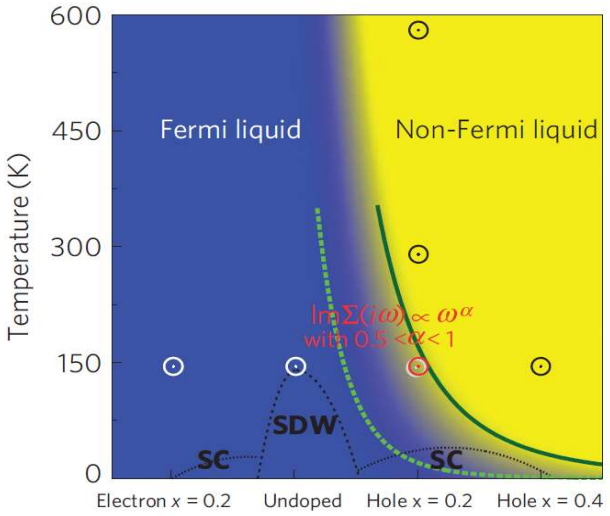


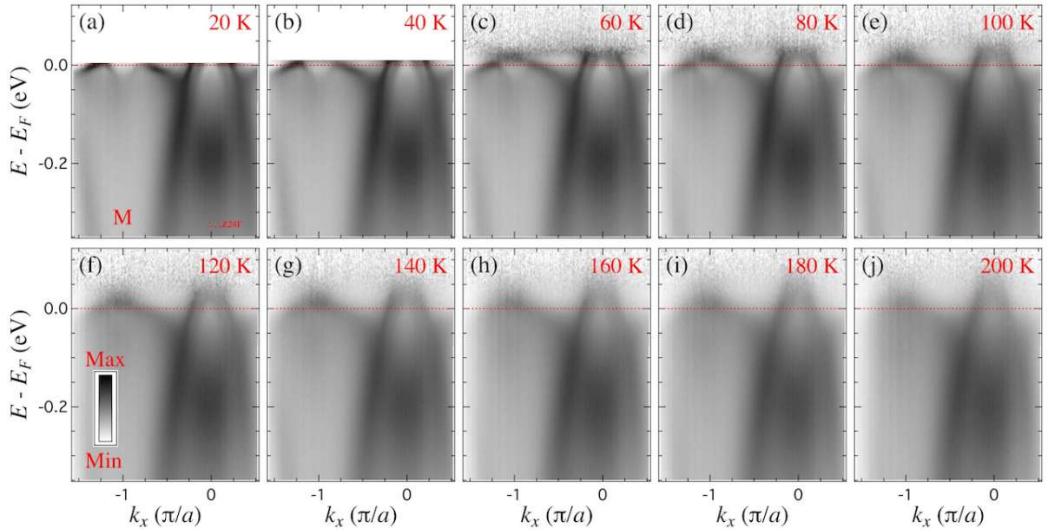
van Roekeghem, Richard, ..., Biermann and Ding, Physical Review B 93, 245139 (2016)

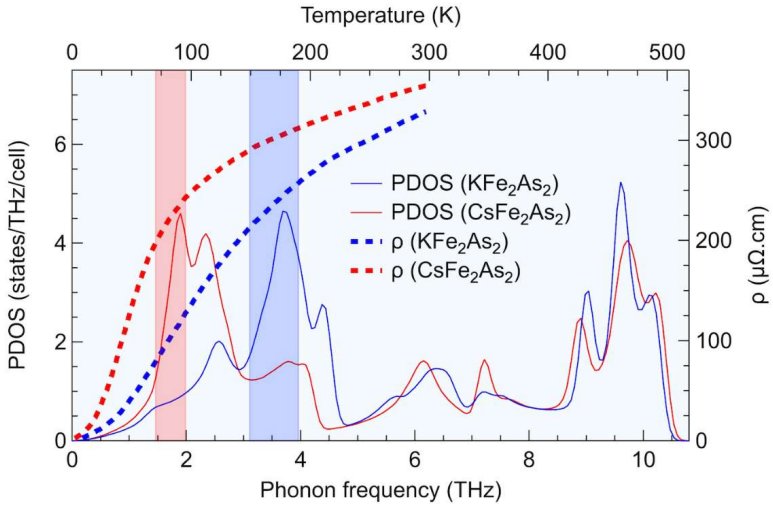
CORRELATIONS OR PHONONS?





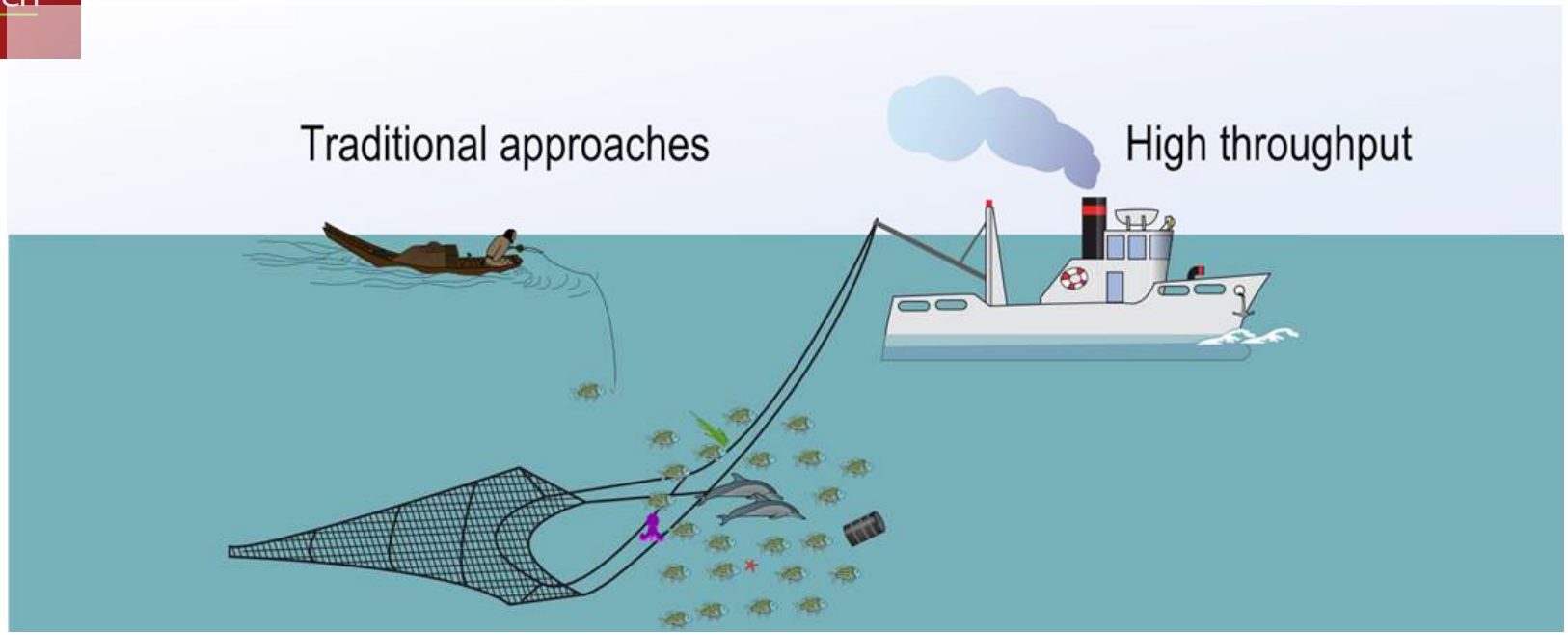






Richard, van Roekeghem, …, Biermann and Ding, arXiv:1807.00193 (2018)

HIGH-THROUGHPUT SCREENING



MATERIALS PROJECT

Energy & Environmental Science — RSC Publishing

PAPER — View Article Online

First principles high throughput screening of oxynitrides for water-splitting photocatalysts

Yabi Wu,[a] Predrag Lazic,[a] Geoffroy Hautier,†[a] Kristin Persson[b] and Gerbrand Ceder*[a]

AFLOW

Automatic - FLOW for Materials Discovery

nature materials — REVIEW ARTICLE

The high-throughput highway to computational materials design

Stefano Curtarolo[1,2]*, Gus L. W. Hart[2,3], Marco Buongiorno Nardelli[2,4,5], Natalio Mingo[2,6], Stefano Sanvito[2,7] and Ohad Levy[1,2,8]

NOMAD

NREL — NATIONAL RENEWABLE ENERGY LABORATORY

High Performance Computing Center
Materials Database

ARTICLES — nature chemistry

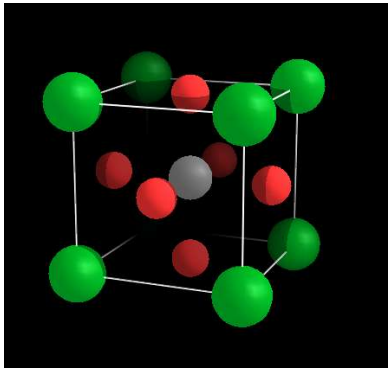
Prediction and accelerated laboratory discovery of previously unknown 18-electron ABX compounds

Romain Gautier[†], Xiuwen Zhang[2†], Linhua Hu[†], Liping Yu[2], Yuyuan Lin[†], Tor O. L. Sunde[†], Danbee Chon[†], Kenneth R. Poeppelmeier[†]* and Alex Zunger[2]*

AiiDA

HIGH-THROUGHPUT SCREENING

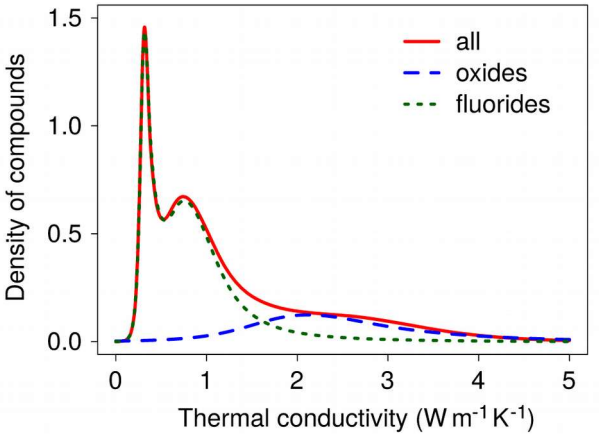
ABX_3 with X=O or F



H																	He
Li	Be											B	C	N	O	F	Ne
Na	Mg											Al	Si	P	S	Cl	Ar
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xn
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn

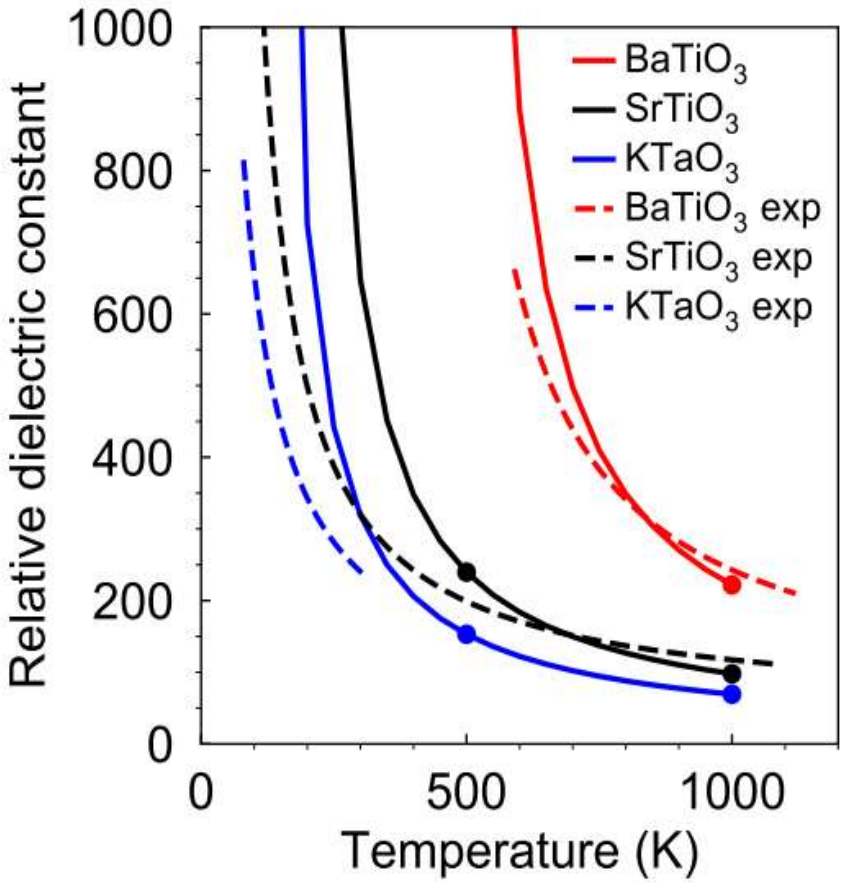
- 8000 possible combinations
- 400 non-magnetic semi-conductors
- 90 found mechanically stable at 1000 K

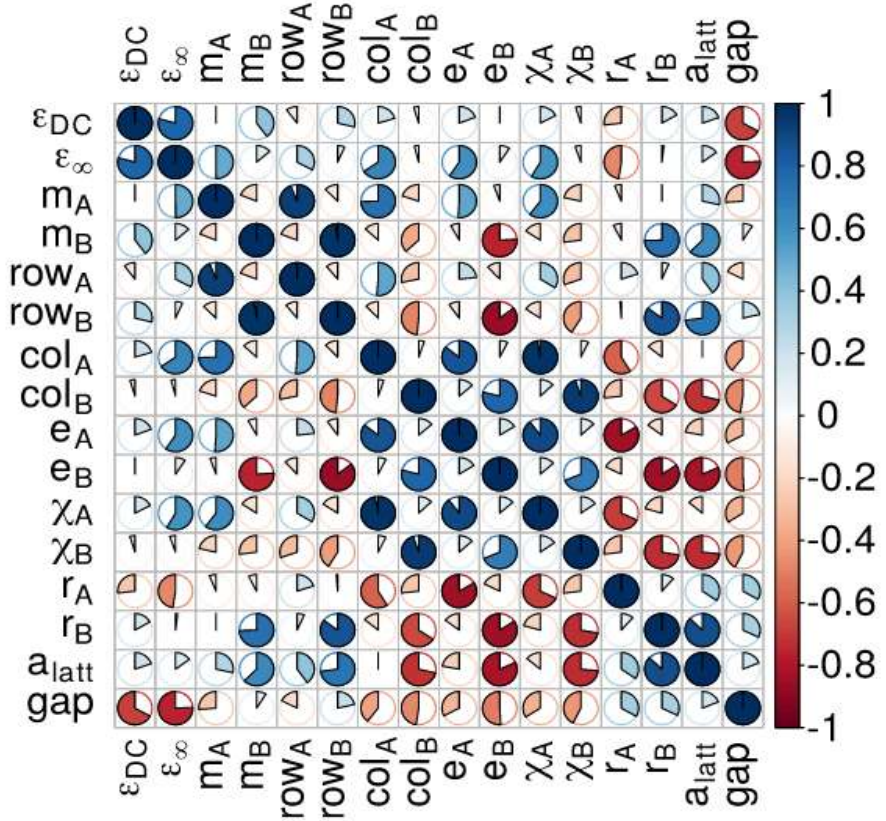
- 35 already synthesized perovskites
- 17 mentioned only as non-perovskites
- 38 potentially new compounds
- 2 with negative thermal expansion at 300 K



van Roekeghem et al., Phys. Rev. X 6, 041061 (2016)

HIGH-THROUGHPUT SCREENING





van Roekeghem, Carrete, Curtarolo and Mingol, arXiv:1805.09199, submitted to PRM (2018)

Thank you!

Commissariat à l'énergie atomique et aux énergies alternatives
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