FROM TRANSITION METAL PNICTIDES TO HIGH-THROUGHPUT COMPUTATIONAL SCREENING

61st anniversary of the Centre de Physique Théorique - 24/03/2019
Ambroise van Roekeghem
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?
SUPERCONDUCTIVITY IN IRON PNICTIDES

DOES IT LOOK GOOD?

Credit: Jeff Fitlow/Rice University
FROM BA0.6K0.4FE2AS2 TO BACO2AS2

Werner et al, Nature Physics 8 (2012): 331
THEORETICIANS DOING EXPERIMENTS
EXPECTED THINGS
UNEXPECTED THINGS
Having 2 advisors, a good idea?
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 Biermann1
1Centre de Physique Théorique, Ecole Polytechnique, CNRS, Université Paris-Saclay, 91128 Palaiseau, France
2Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany
3Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

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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$^{1(*)}$, 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$^{1(b)}$

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Electronic Band Structure of BaCo$_2$As$_2$: 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

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Having 2 advisors, a good idea?

Screening of Coulomb interaction

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

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

\[ \tilde{H}_{\text{loc}} = (V - 2 \frac{\lambda^2}{\omega_0}) \tilde{n}_{\uparrow} \tilde{n}_{\downarrow} \]
\[ - \frac{\lambda^2}{\omega_0} (\tilde{n}_{\uparrow} + \tilde{n}_{\downarrow}) + \omega_0 \left( b^\dagger b + \frac{1}{2} \right) \]
The SEX+DDMFT method

WHERE IS MASSIMO?
Computing Phonons

Quantum statistics, finite T

\[ \rho_{h}(\{u_{i\alpha}\}) \propto \exp\left(-\frac{1}{2} u^{T} \Sigma^{-1} u \right) \]

\[ \Sigma(i\alpha, j\beta) = \frac{\hbar}{2\sqrt{M_i M_j}} \sum_{m} \omega_{m}^{-1}\left[1 + 2n_{B}(\omega_{m})\right] \epsilon_{m\alpha} \epsilon_{m\beta}^{*} \]

CORRELATIONS OR PHONONS?


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

HIGH-THROUGHPUT SCREENING
**HIGH-THROUGHPUT SCREENING**

$\text{ABX}_3$ with $X=\text{O}$ or $\text{F}$

- 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

Thank you!