Disentangling the mechanism of unconventional superconductors using high performance computing

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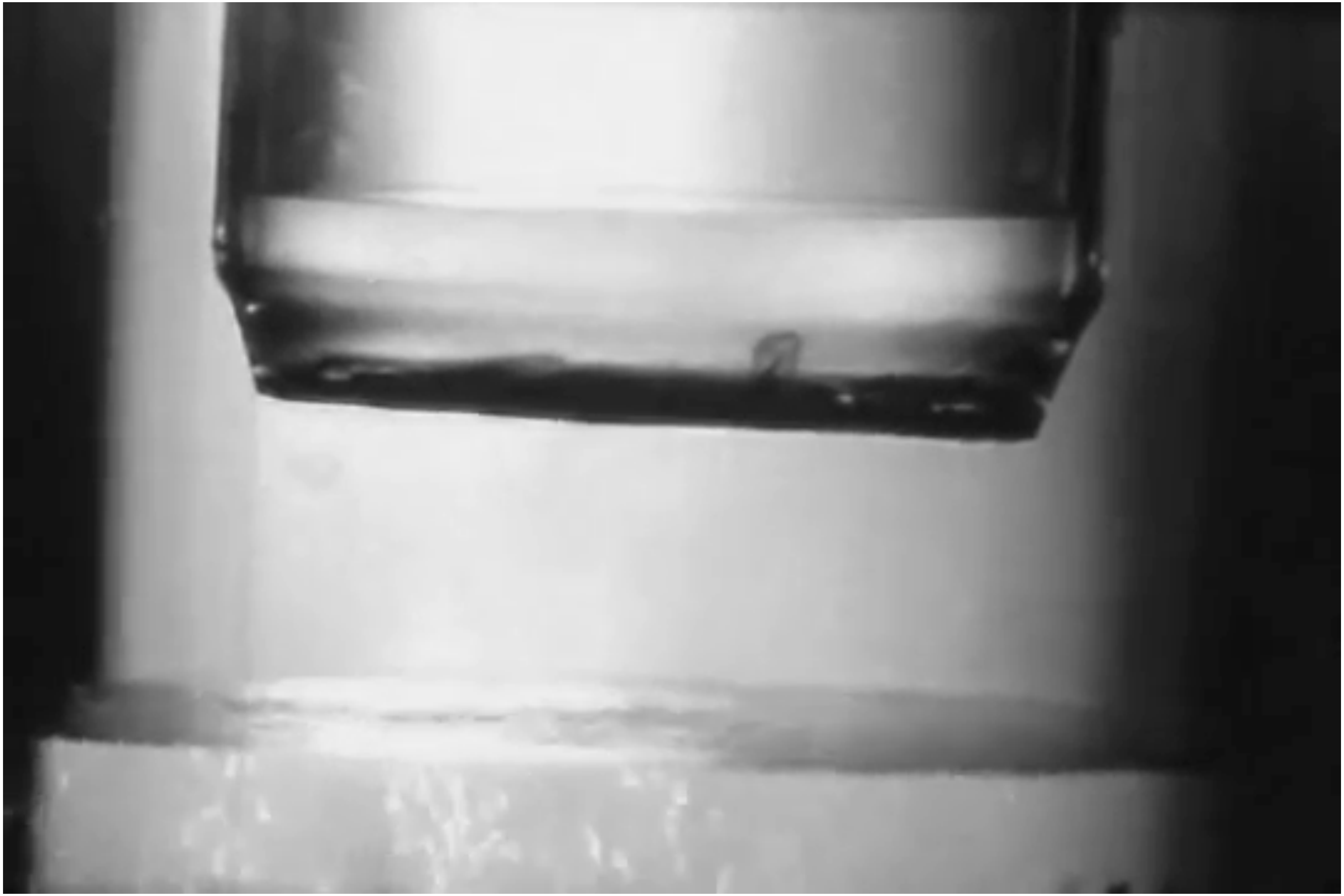
arXiv:1705.01008

Superfluid



Alfred Leitner

Superconductor: superfluid of electrons

5,570 amps through a lamp cord!

5% of our power is lost through transmission. (eia.gov)

With superconductors, that could be ~0%

MRI, sensors, electric motors, …

Superconductivity is caused by pairing

Bardeen, Cooper, Schreiffer

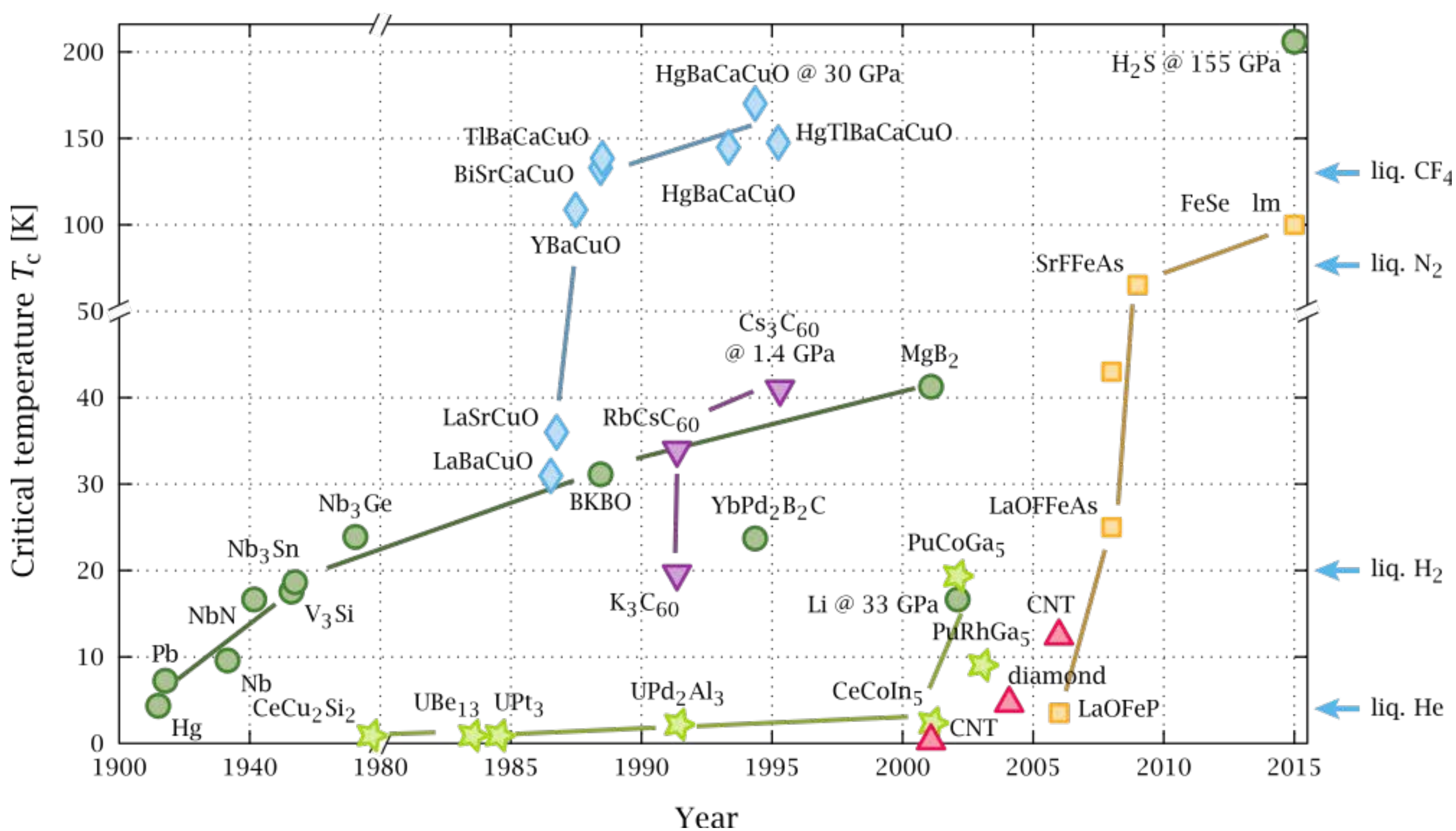
Two types of superconductivity

Conventional:

- Common
- Low temperature / high pressure
- ‘Wakes’ in the atomic lattice

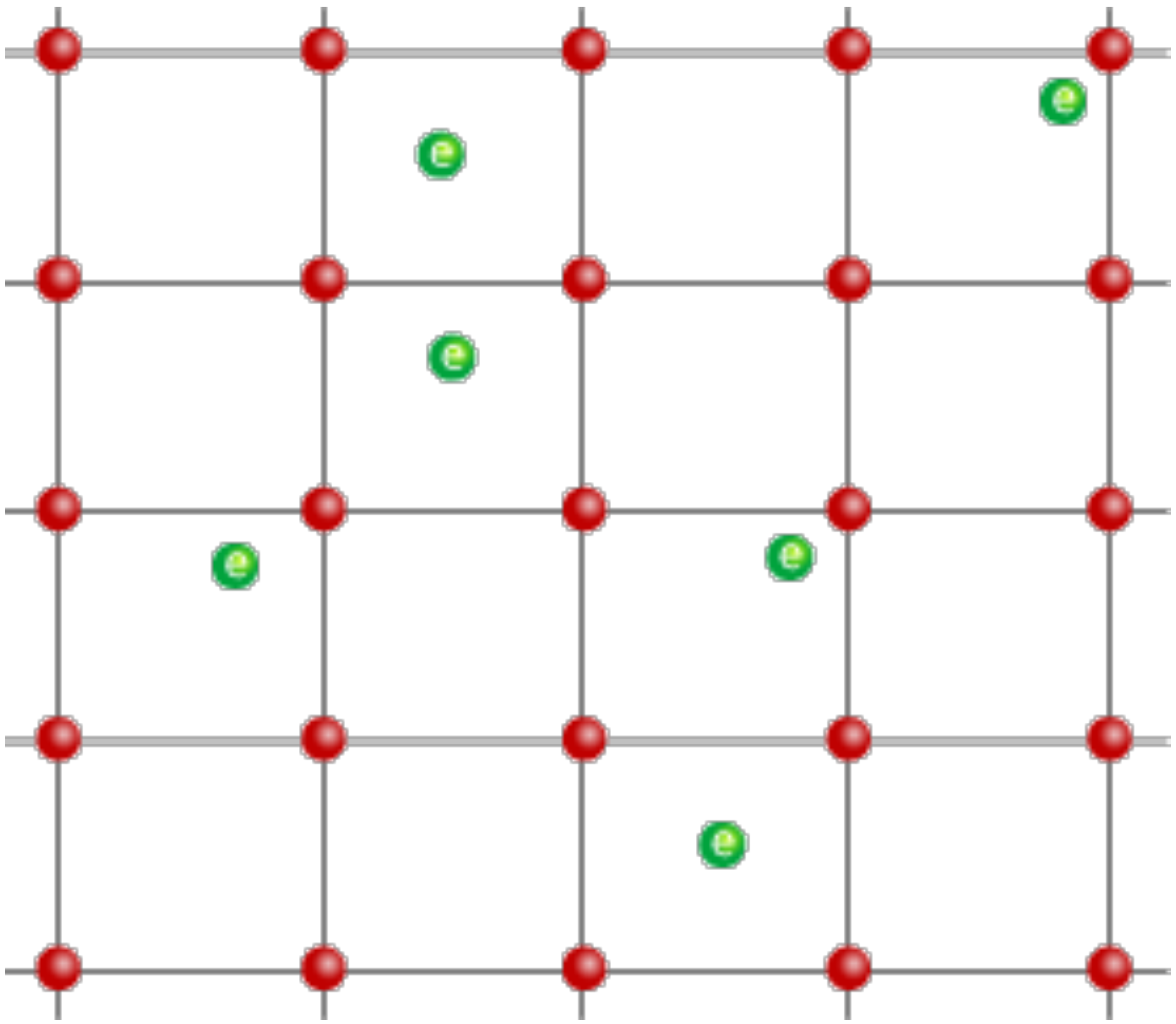
Unconventional

- Rare
- High temperature
- **Origin unknown**

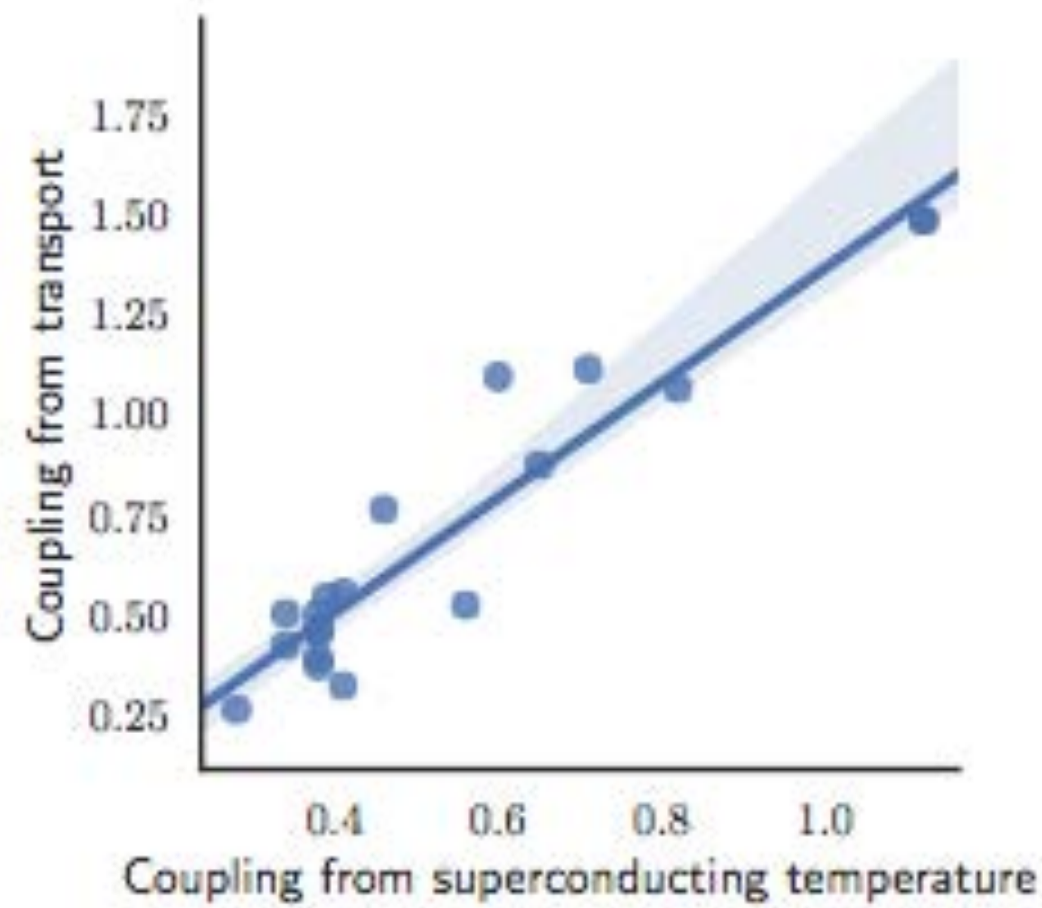


Superconductivity—very common

Conventional superconductors



Attraction due to the lattice of nuclei



Data from Philip B. Allen “The electron-phonon coupling constant lambda”

http://lrrpublic.cli.det.nsw.edu.au/lrrSecure/Sites/Web/physics_explorer/physics/lo/superc_03/superc_03_00.htm

Unconventional superconductors??

Given A,B,C,D, what is the probability that the material is superconducting?

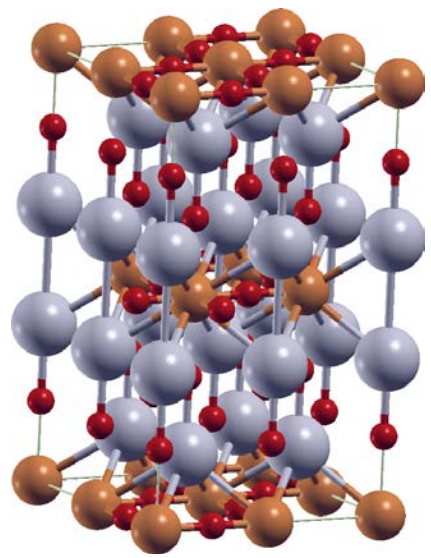
$$P(\text{superconducting}|A, B, C, D)$$

Probability function

Computed accurately for a given material

Need to compute A, B, C accurately and compare to experimental observations

Many particle quantum mechanics

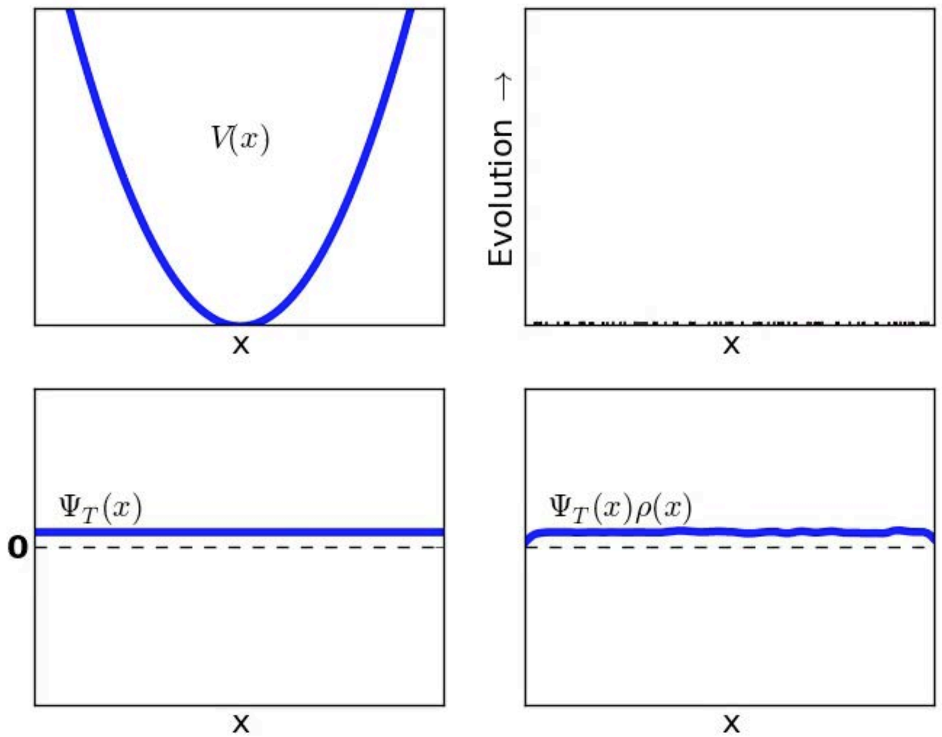
Start with  + $\hat{H} = -\frac{1}{2}\sum_i \nabla^2 - \sum_{i\alpha}\frac{Z_\alpha}{r_{i\alpha}} + \sum_{ij}\frac{1}{r_{ij}} + \sum_{\alpha\beta}\frac{Z_\alpha Z_\beta}{r_{ij}}$

No effective parameters

Solve $E_i\Psi_i(r_1, r_2, \ldots) = \hat{H}\Psi_i(r_1, r_2, \ldots)$

Minimal approximations including electron correlations explic

Diffusion Monte Carlo

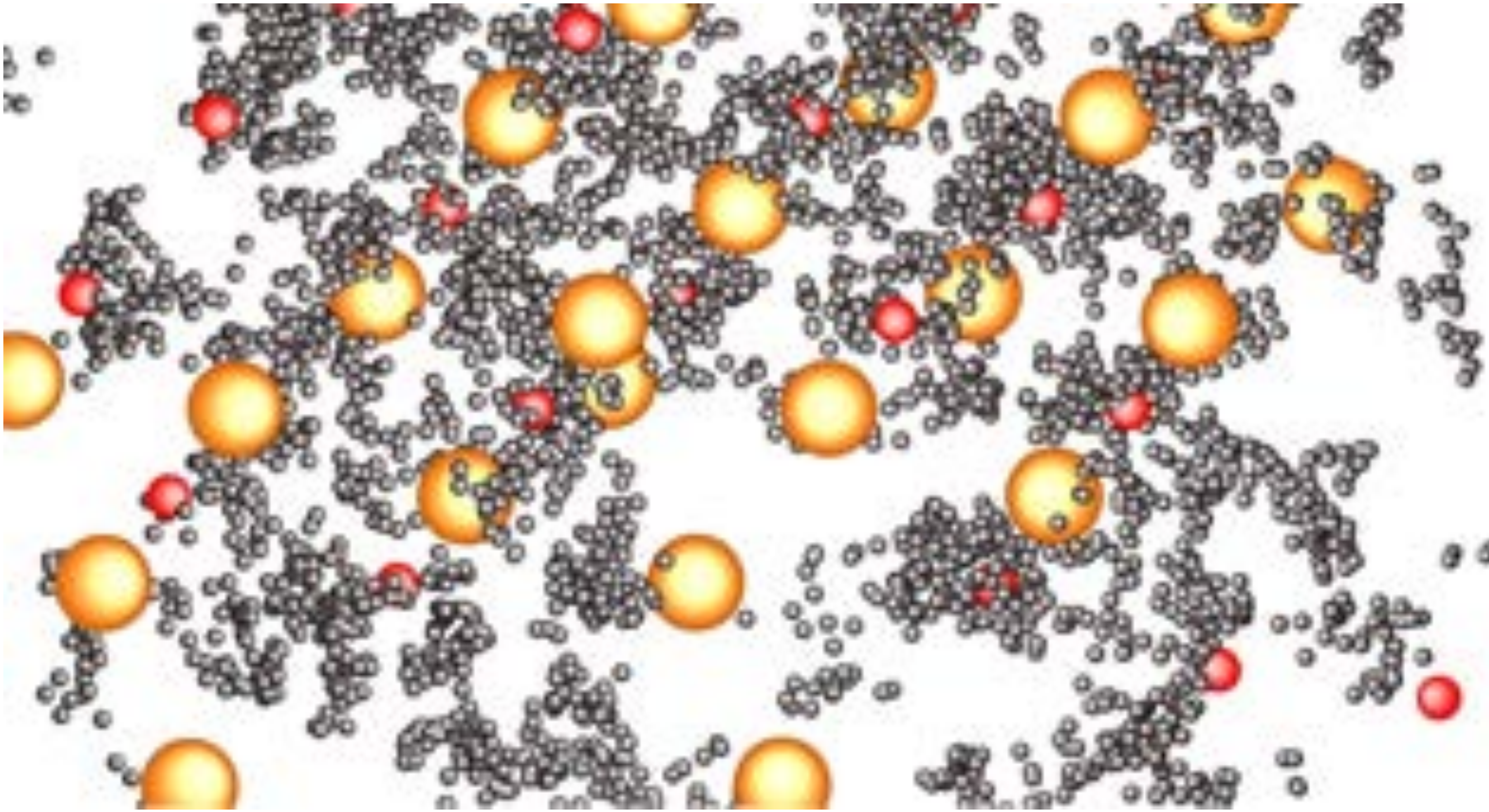


Stationary Schroedinger equation
<-> stochastic process

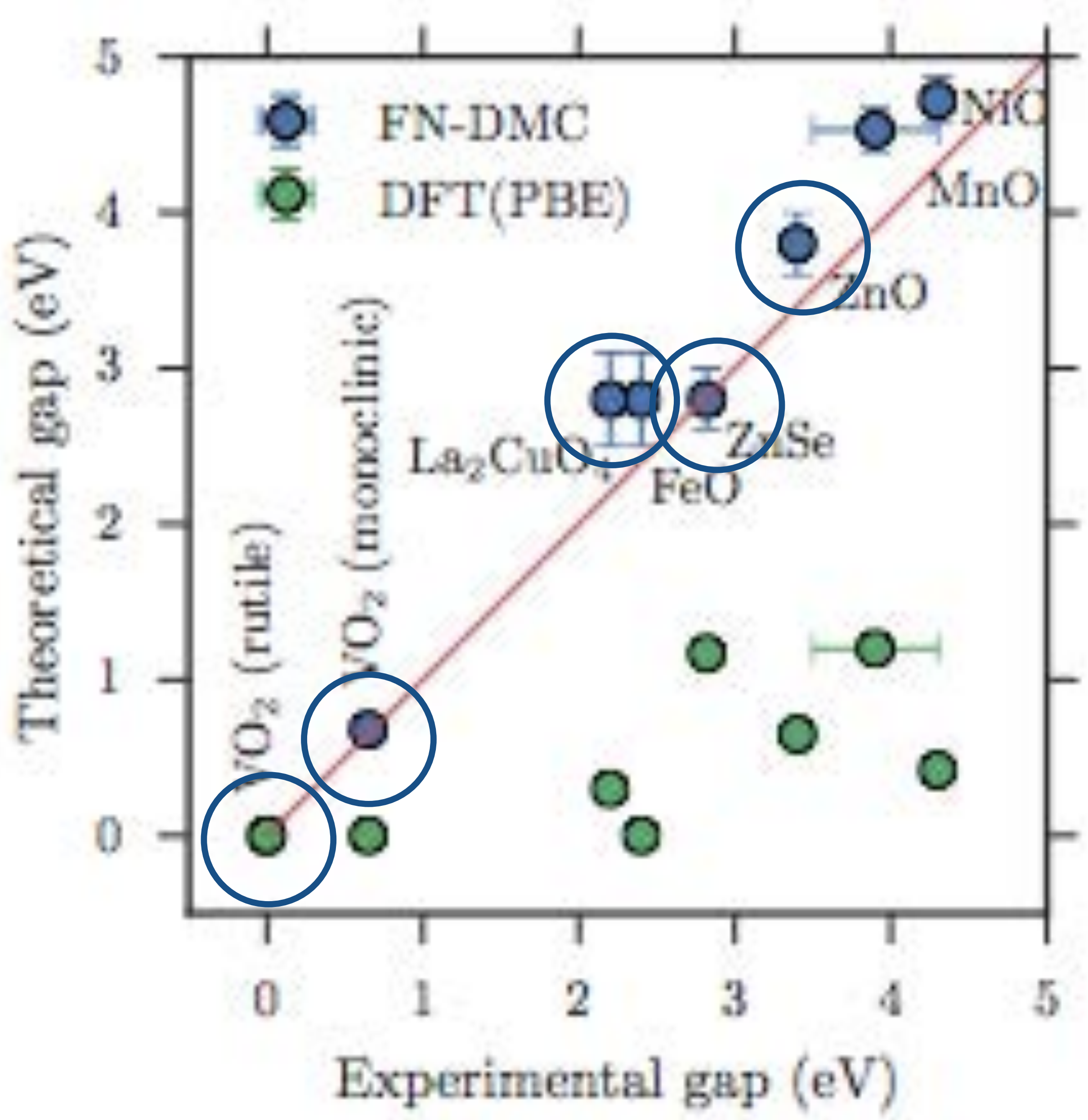
Two mild approximations:

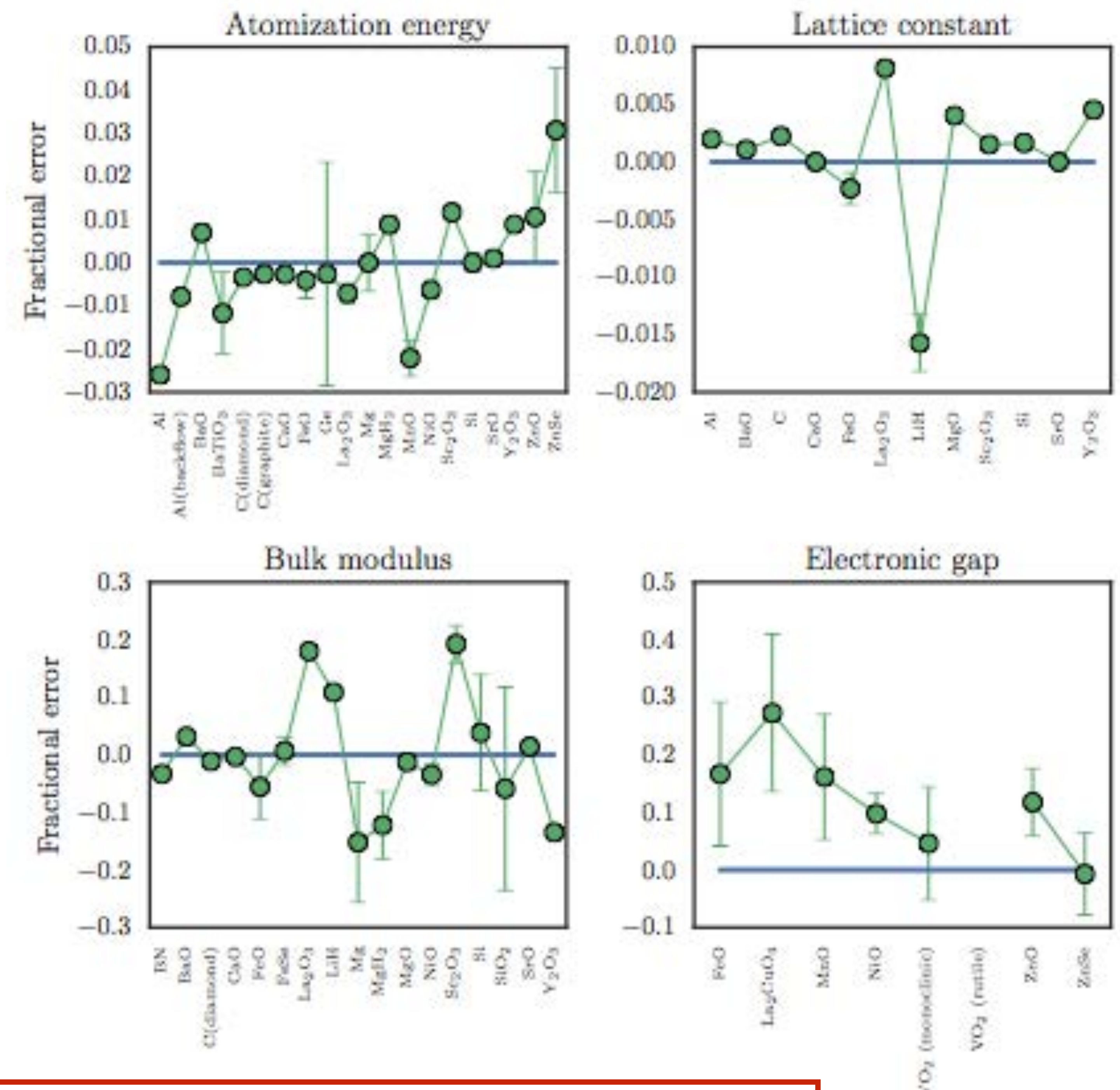
- Fixed node
- Effective core potentials

Realistic simulations



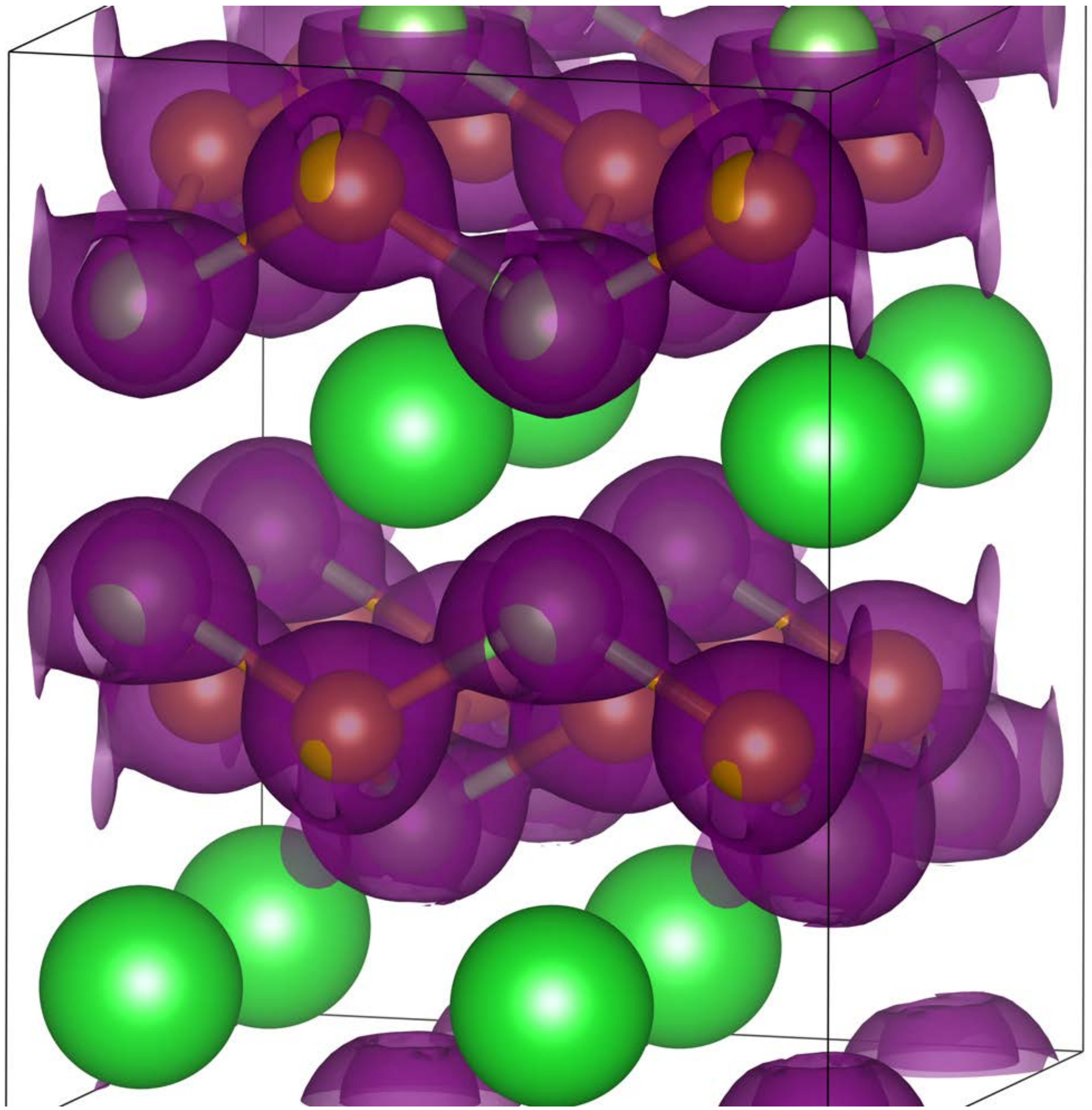
Accuracy of QMC





Each of these points is often one HPC project!

Computational experiment

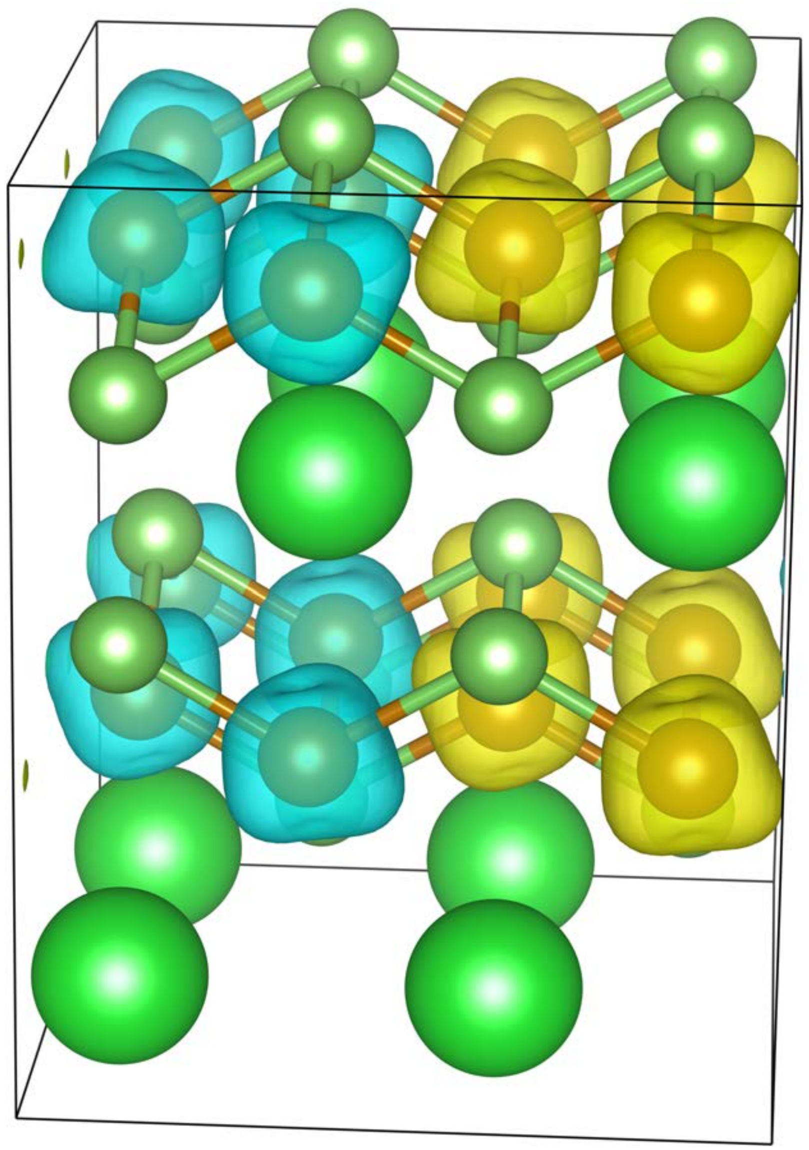


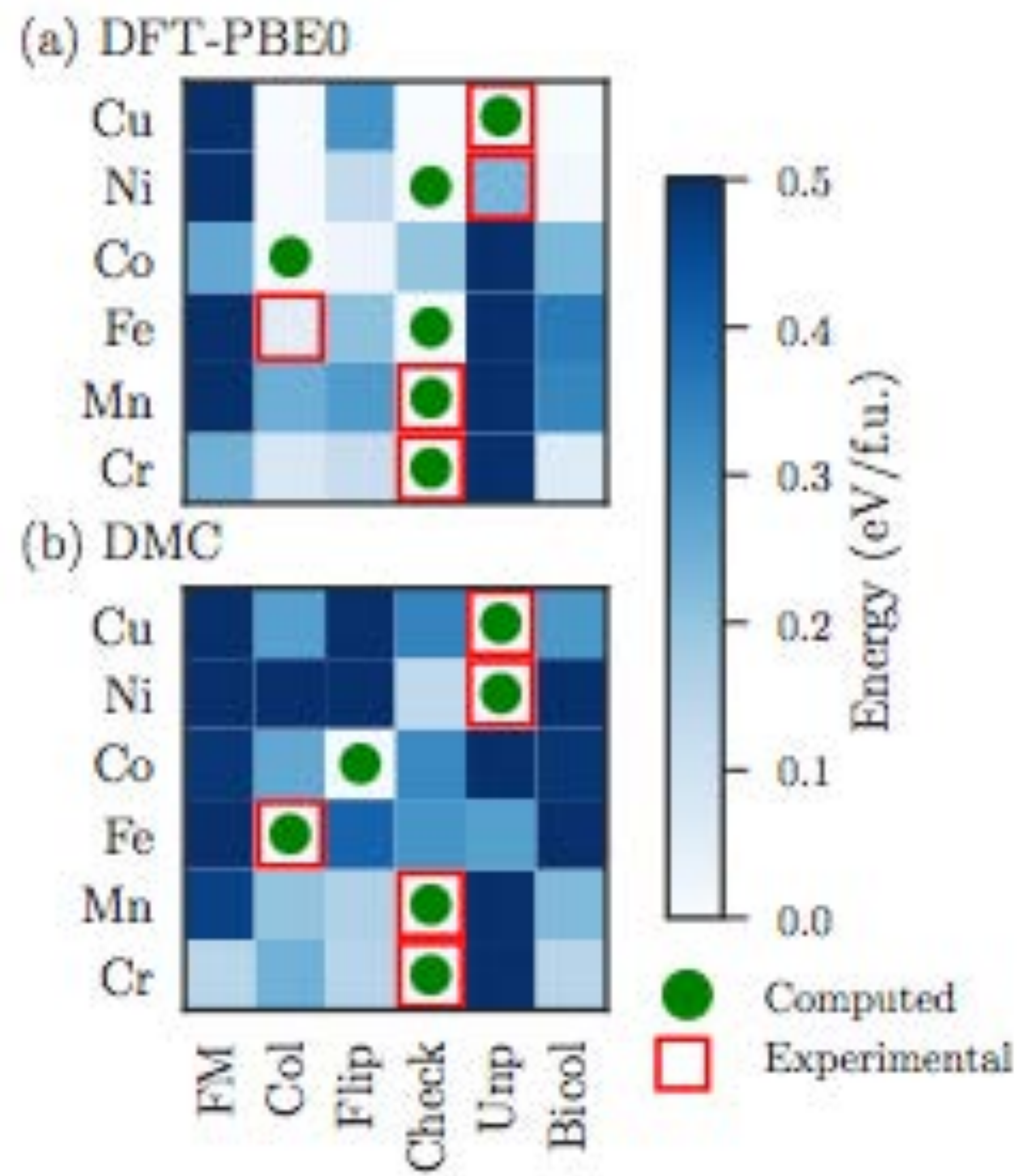
BaM_2As_2
Can make it with
Cr,Mn,Fe,Co,Ni,Cu

Only superconducts with Fe!

Why?

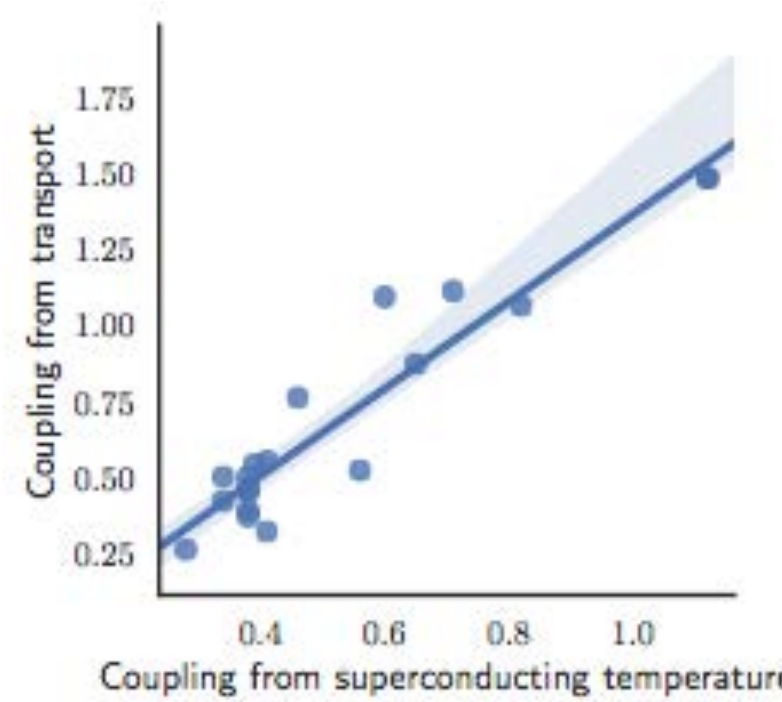
Magnetism in our test set

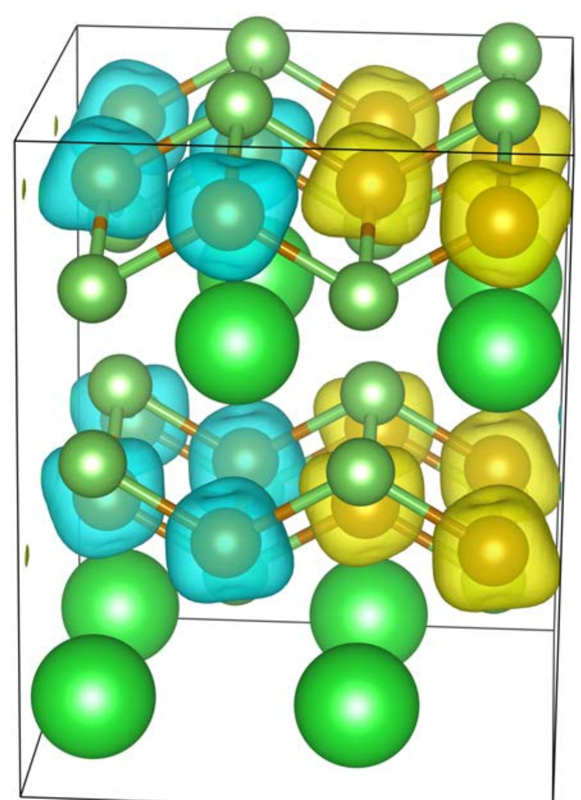




Perfect accuracy on the lowest energy magnetic ordering of these materials

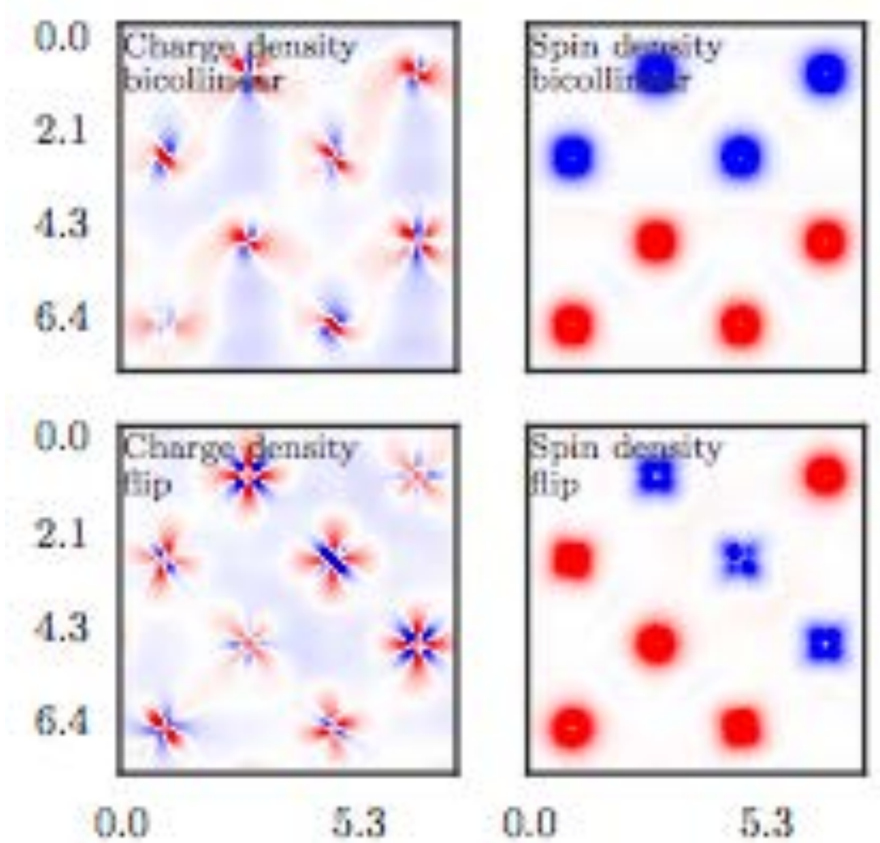
Descriptor for unconventional superconductors



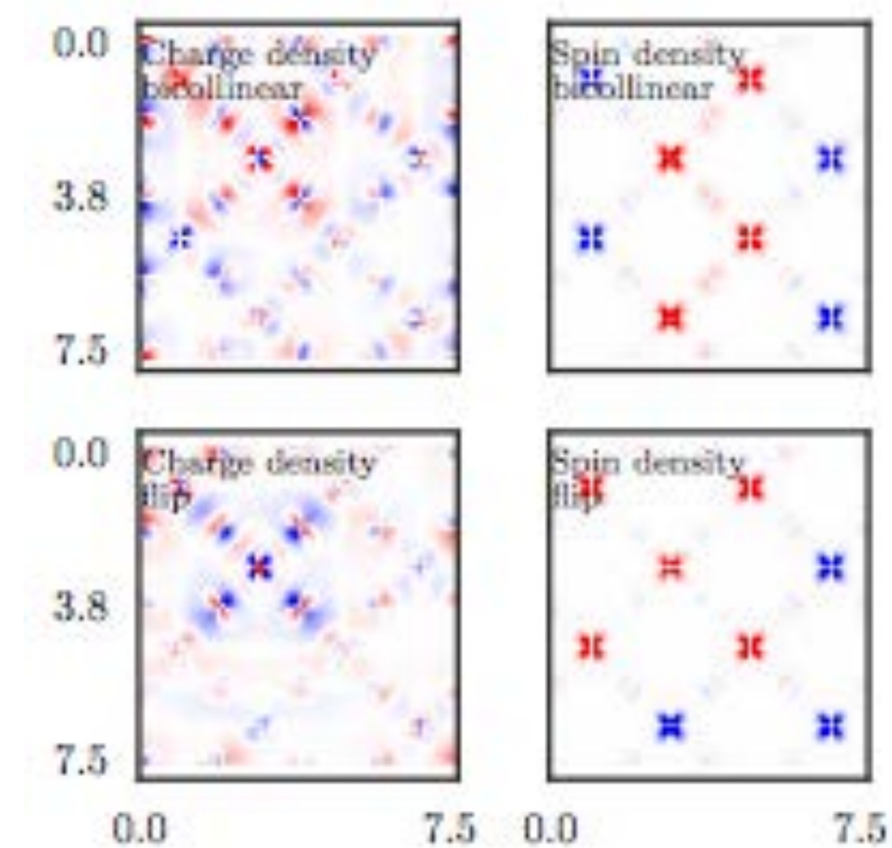


Interactions between charge and spin

$BaFe_2As_2$



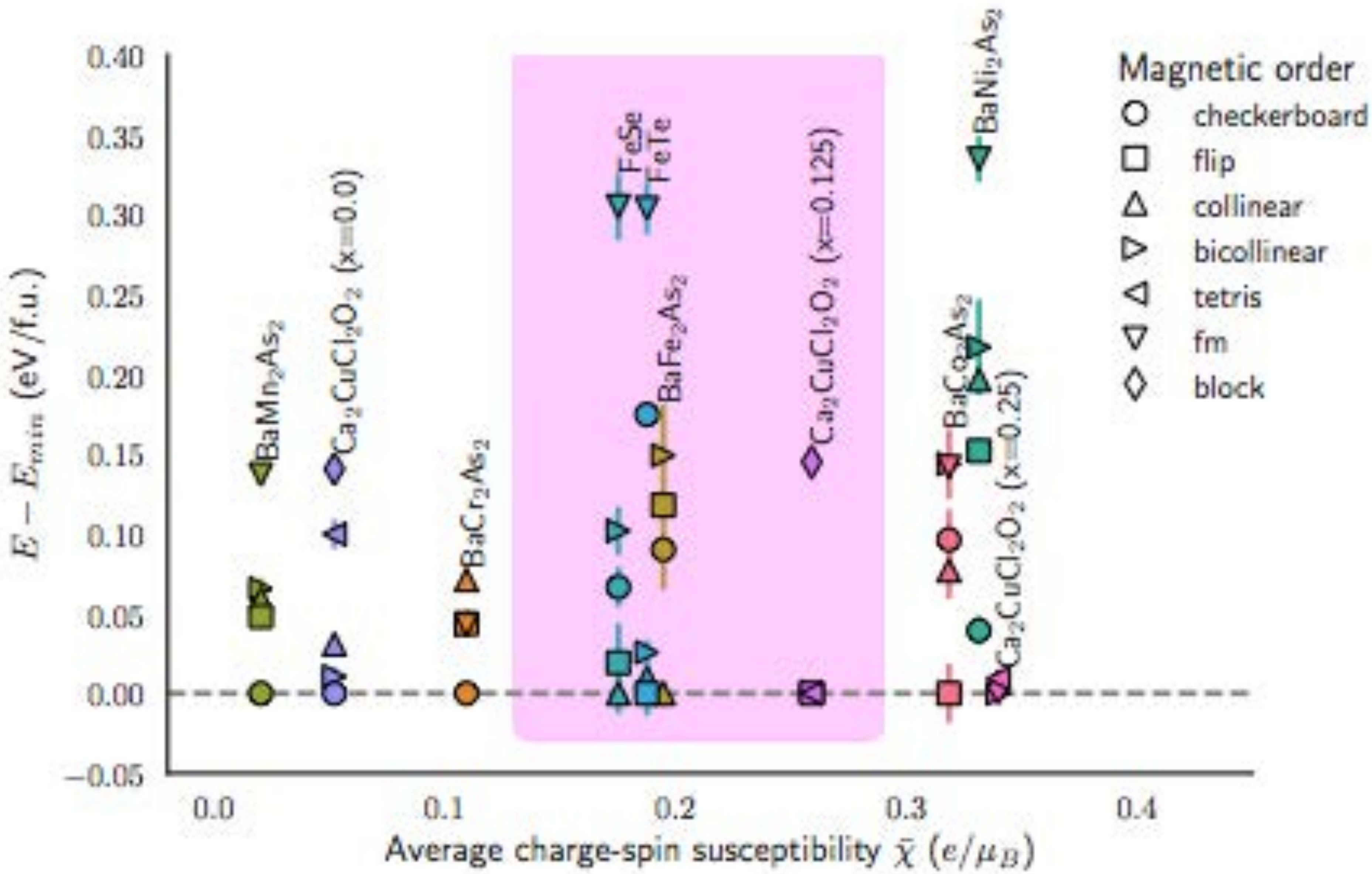
$Ca_2CuO_2Cl_2$ (1/8 doped)



Changing spins -> changes density in superconductors

For more info on this idea, see: Scalapino. Rev. Mod. Phys. 84 1383 (2012)

A sweet spot for unconventional superconductivity



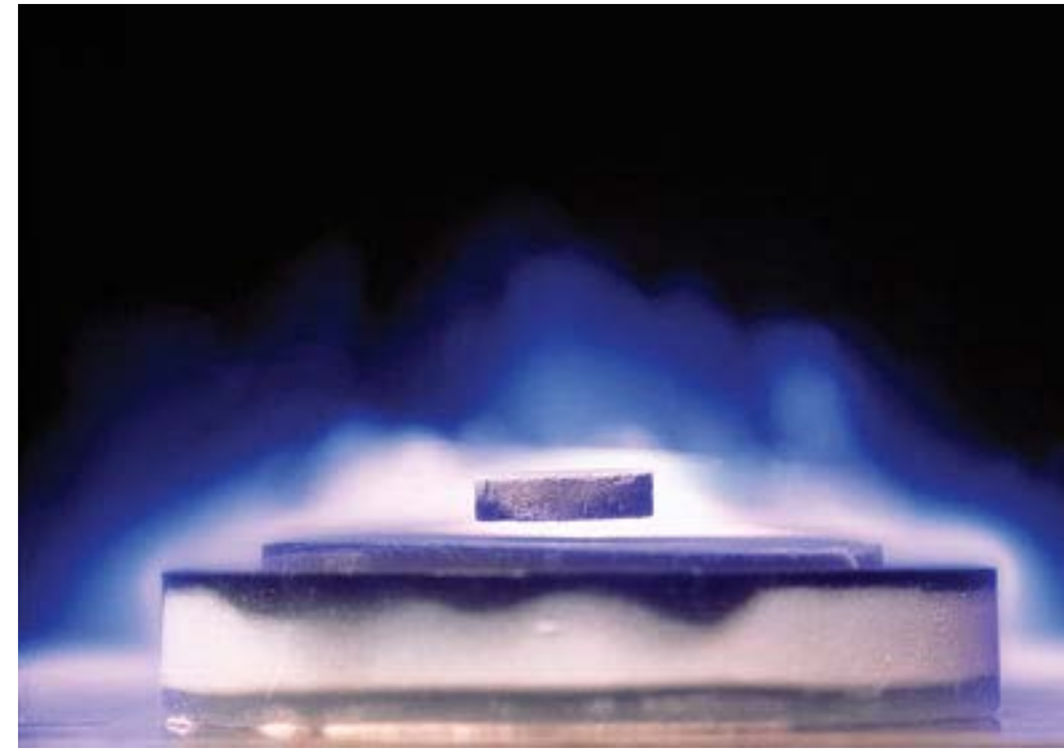
$$\bar{\chi} = \frac{\text{change in density}}{\text{change in spin}}$$

Summary

Connection between atomic scale and emergent behavior

High performance necessary to study many materials

Data will be available through Materials Data Facility



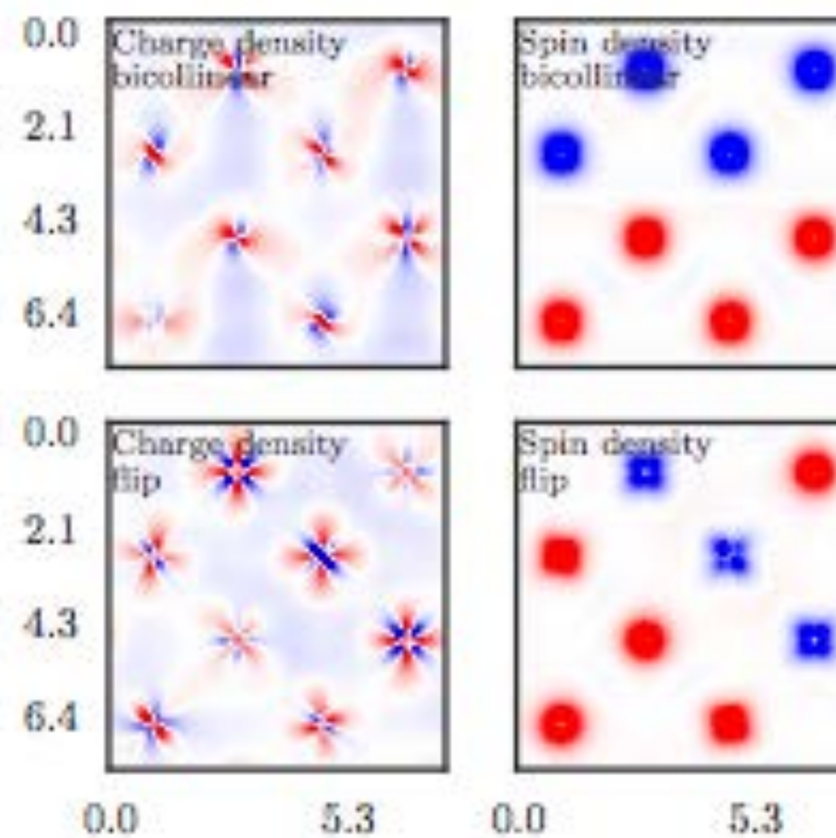


Photo from *Nature* **443**, 376-377

Computational and data challenges

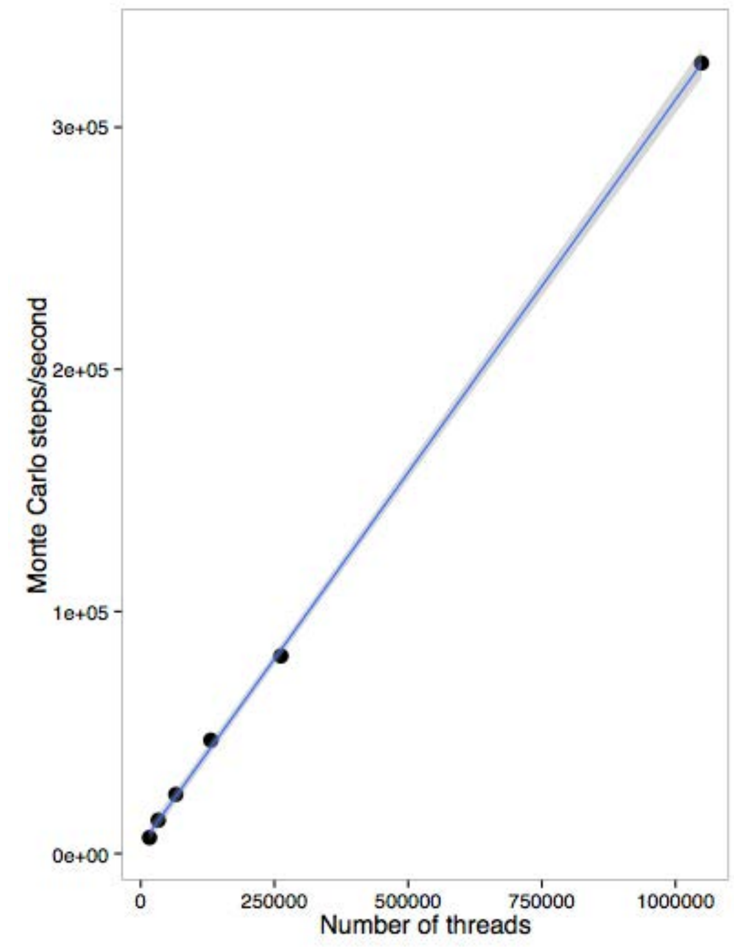
Monte Carlo-scale to 1,000,000 threads easily.

Billions of small matrix operations: ~200-500 elements.

High throughput very desirable to answer physical questions.

Workflow is complex—working on better tools with NCSA & Elif Ertekin

Feature extraction — compute emergent properties from first principles using ML techniques.



www.qwalk.org