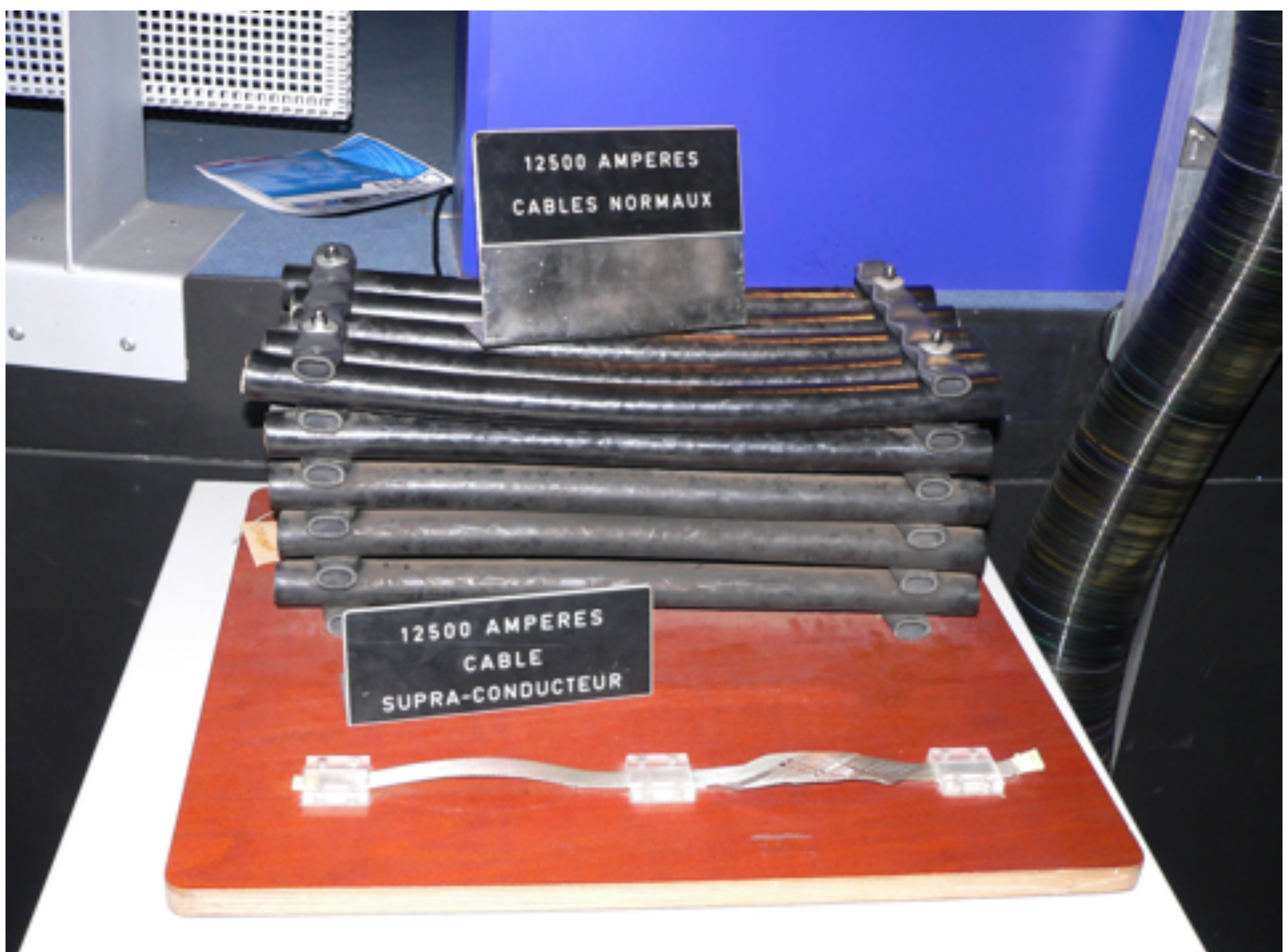
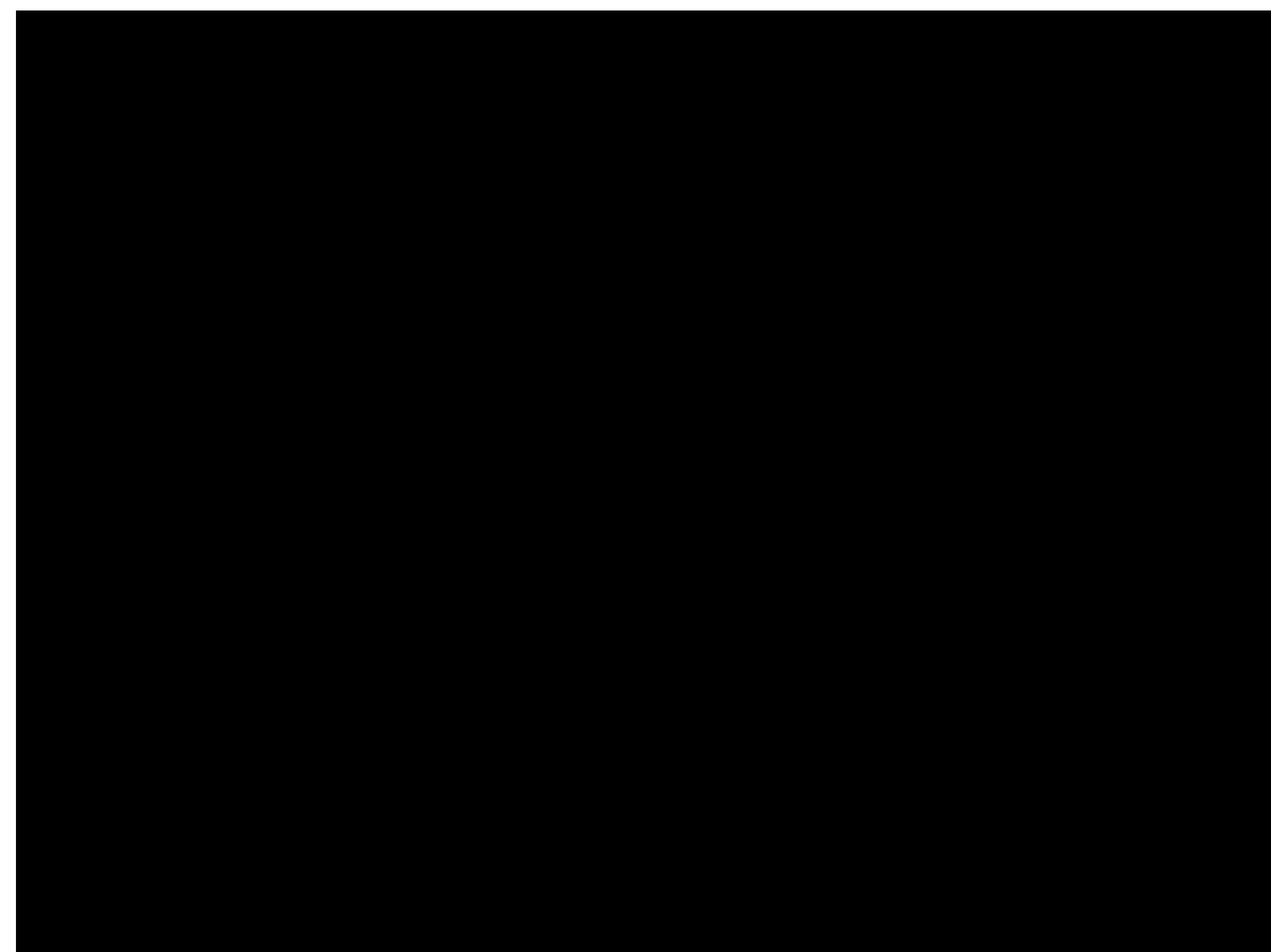
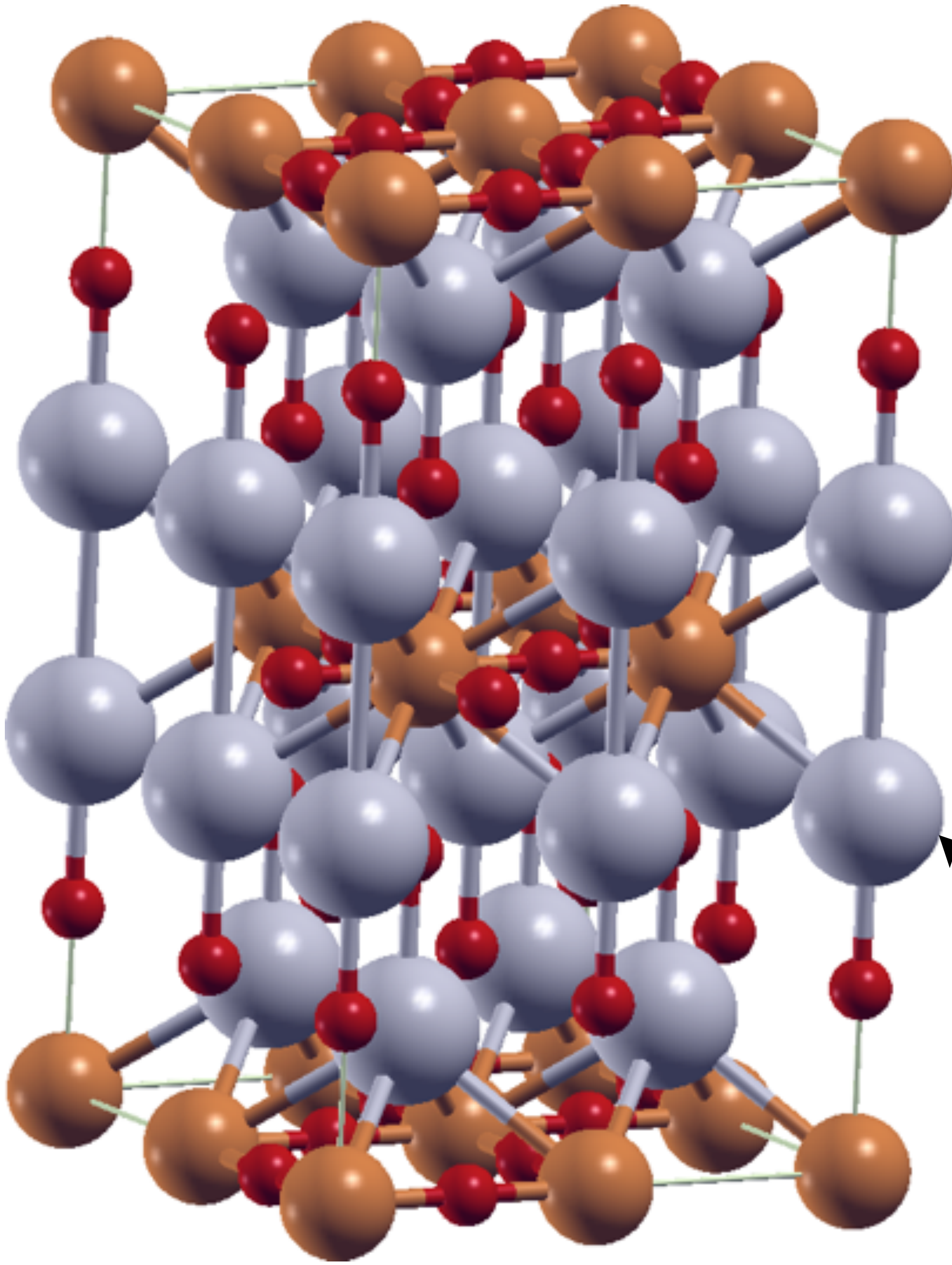
# Computational Exploration of Unconventional Superconductors Using Quantum Monte Carlo

Project PI: Lucas K. Wagner



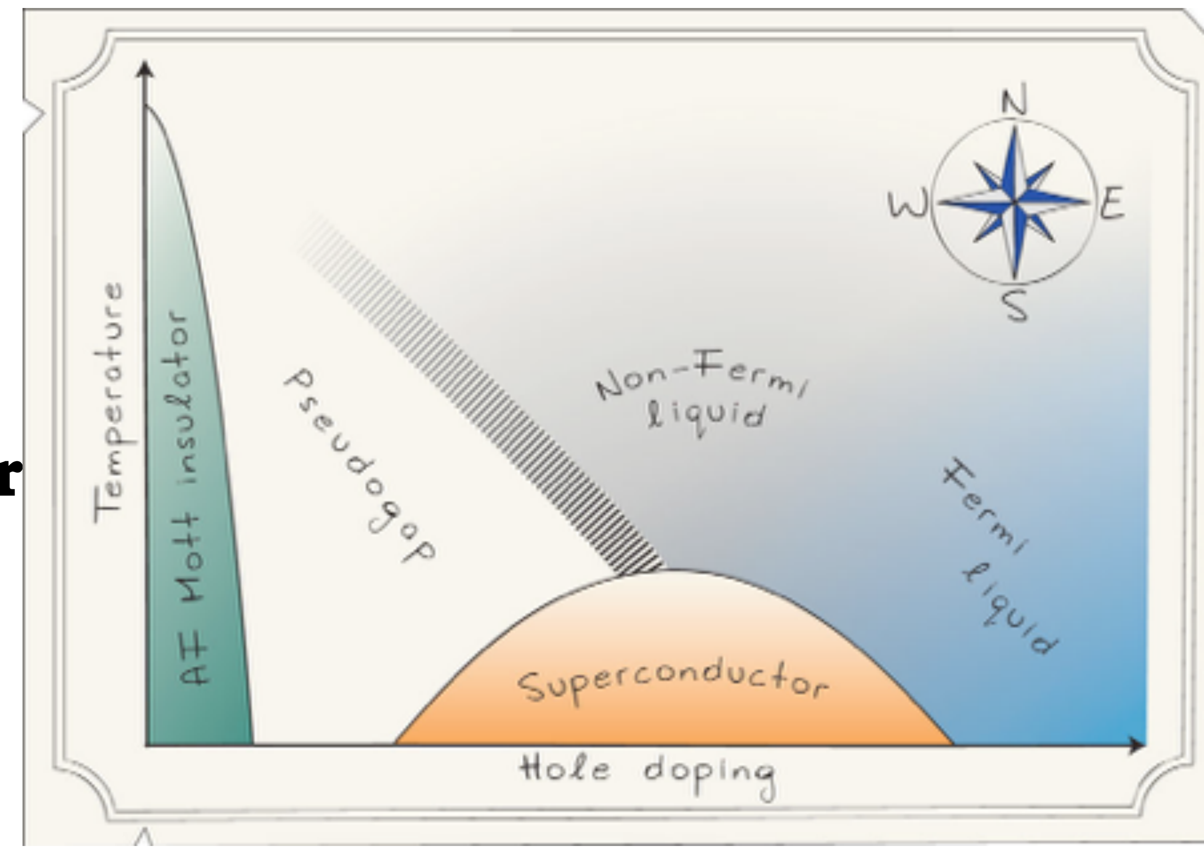
# $La_{2-x}Sr_xCuO_4$ (LSCO) crystal structure



**$CuO_2$ plane**

**LaO ‘spacer**

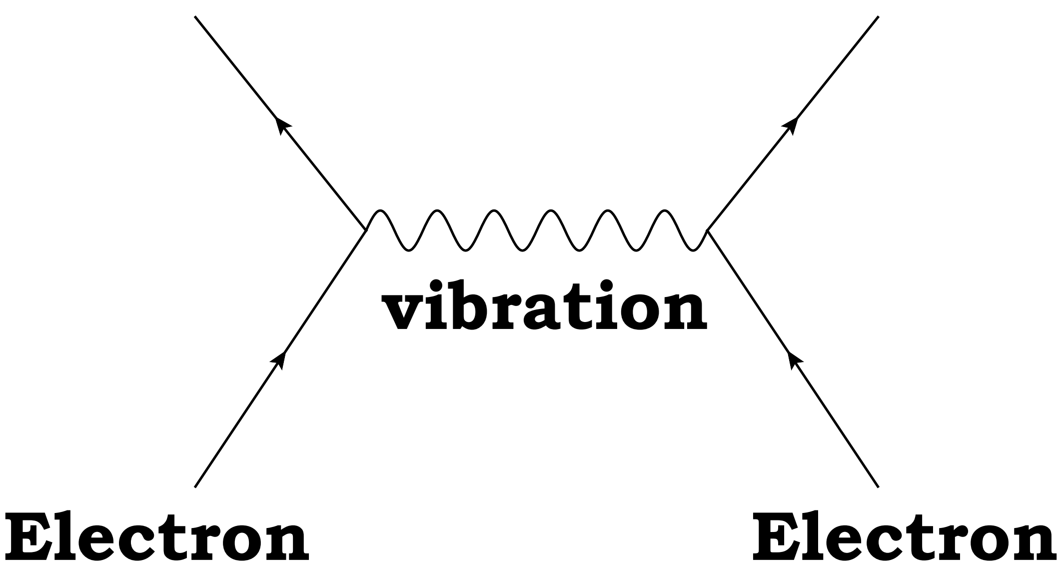
**Doping: La-> Sr**



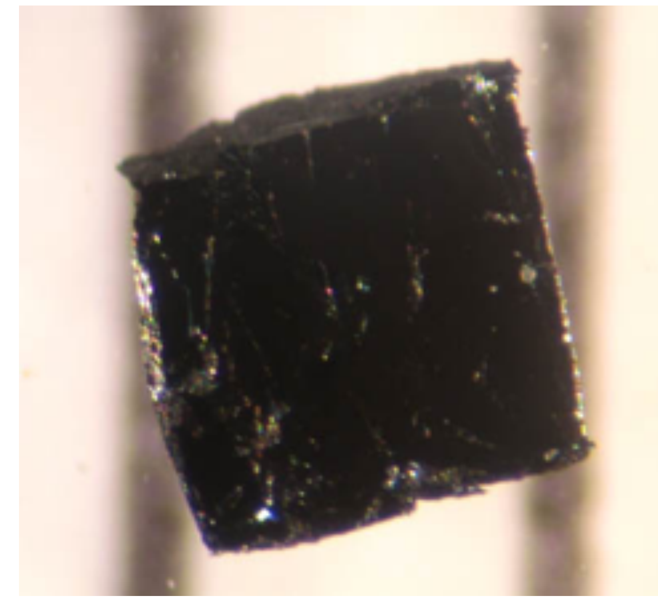

Peter Wahl. Nature Physics 8, 514–516 (2012)

# Contrasting high Tc with low Tc

**Low Tc**
**Maximum theoretical temperature of ~30 K**




**High Tc**
**Maximum observed temperature of ~150 K**



**Electron lattice interactions not enough**

**Possibility of an emergent state from electron-electron interactions**

# Explore La-Cu-O ternary system

| Material ID | Chemical formula | Space group | Formation Energy (eV) | E above Hull (eV) | Band Gap (eV) | Select |
|---|---|---|---|---|---|---|
| mp-3474 | $LaCuO_3$ | $R\bar{3}c$ | -2.4403 | 0 | 0 | |
| mp-20072 | $LaCuO_2$ | $R\bar{3}m$ | -2.7056 | 0 | 2.5 | |
| mp-9416 | $La(CuO_2)_2$ | $I4_1/a$ | -2.0543 | 0 | 0 | |
| mp-5696 | $La_2Cu_2O_5$ | Pmcb | -2.5397 | 0.0484 | 0 | |
| mp-36480 | $La_2CuO_4$ | Ccme | -3.0029 | 0.0518 | 0.3 | |
| mp-654033 | $La_2Cu_2O_5$ | C2/c | -2.5231 | 0.065 | 0 | |
| mp-20574 | $La_2CuO_4$ | I4/mmm | -2.9895 | 0.0652 | 0.2 | |

Selected structures: Edit in XtalToolkit

**Density functional theory $La_2CuO_4$: nonmagnetic, small to no gap, and unstable.**

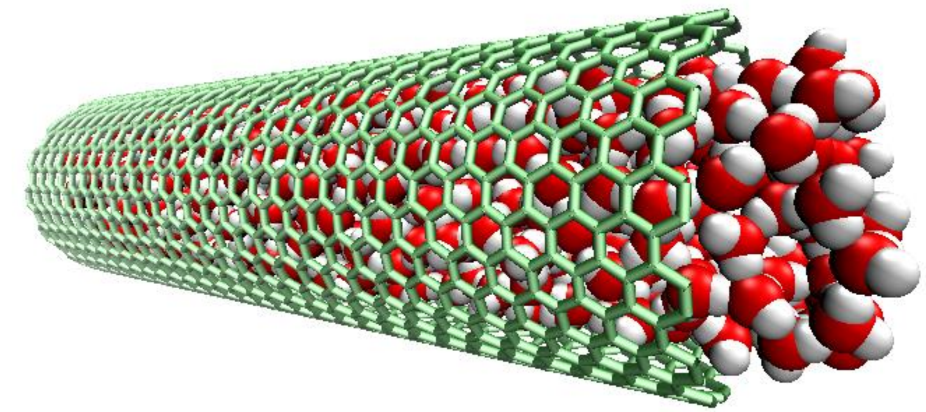
**Need better simulations to successfully predict properties of strongly correlated materials!**

**materialsproject.org**

**Superconductivity is a macroscopic quantum phenomenon. Same equation describes this, and many others.**

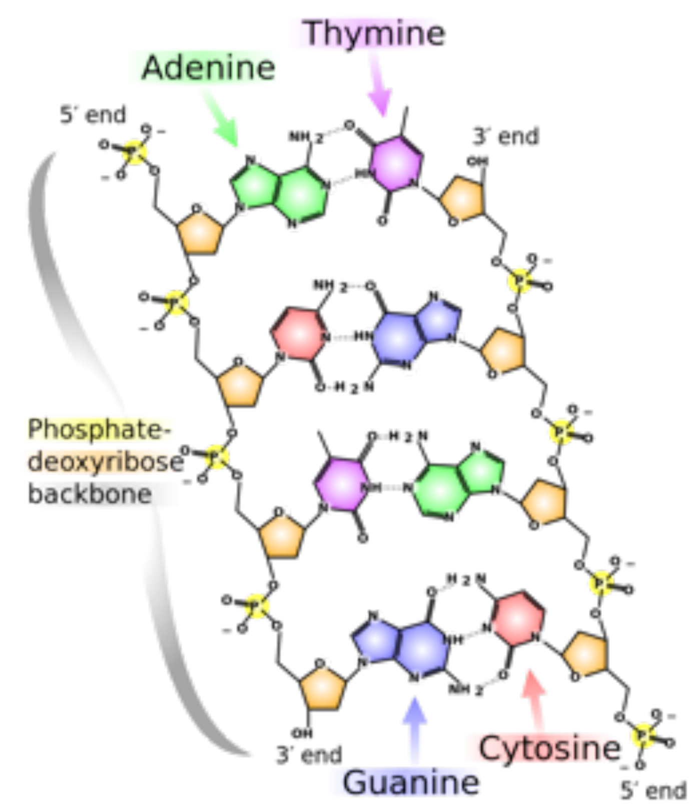
$$i\frac{\partial}{\partial t}\Psi(r_1, r_2, \ldots) = \hat{H}\Psi(r_1, r_2, \ldots)$$

**Differential operator**



**Nanofluidics**

**Advanced solar cells**




**DNA**

# The many-body quantum challenge

**Solve for stationary states**

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

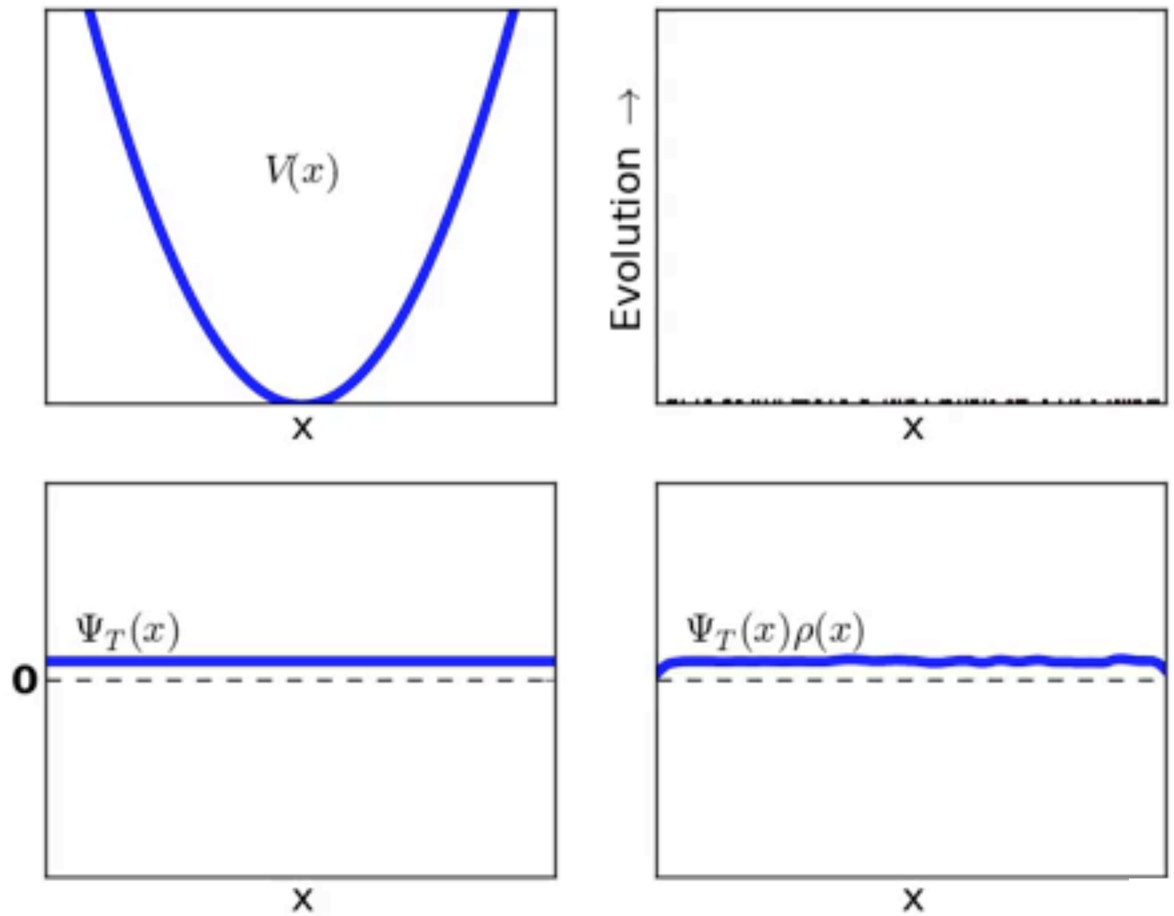
**Position of each particle (electron)**

**This is hard because the wave function is not factorizable!**

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

**Kinetic energy** | **Electron-nucleus** | **Nucleus-nucleus** | **Electron-electron**

**Separable (non-interacting) part** | **Interacting part**




**Diffusion Monte Carlo**

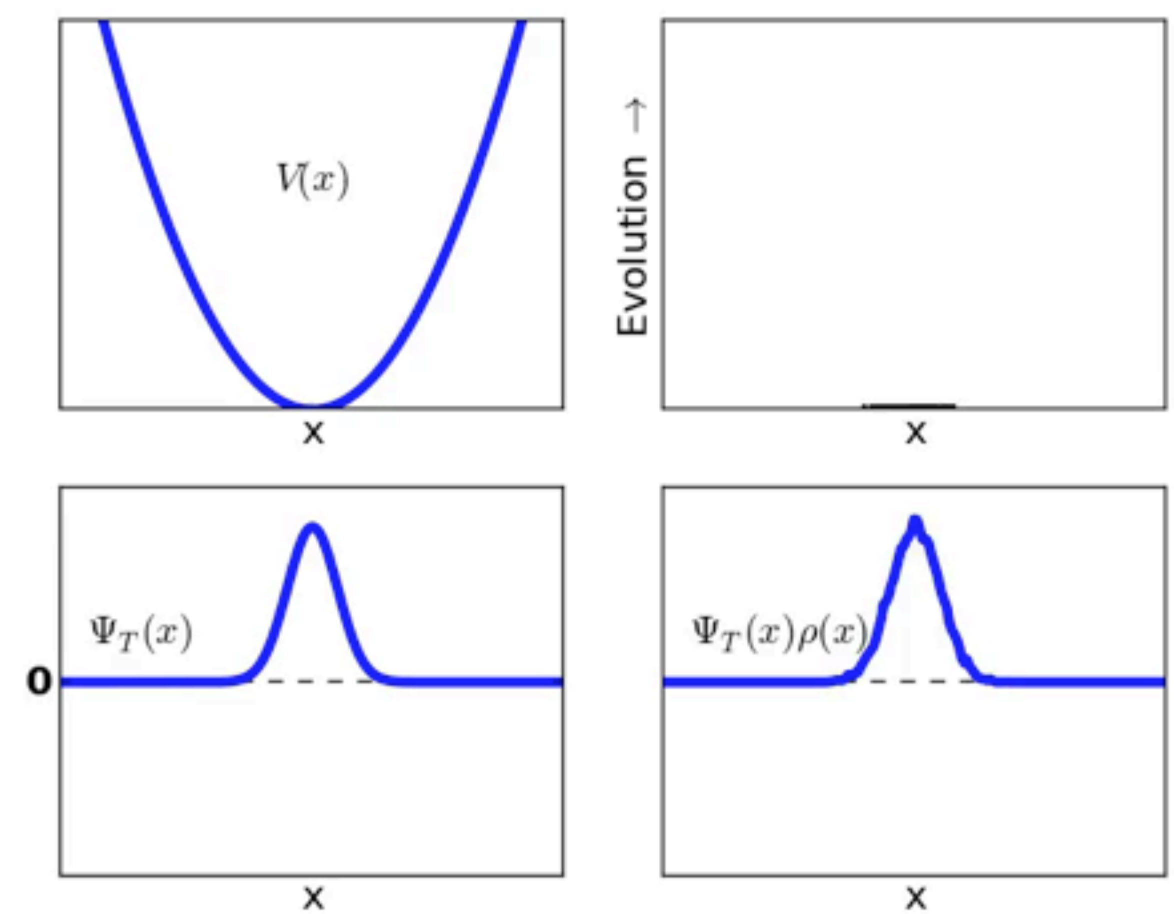
**Isomorphism between stochastic process and stationary Schrodinger equation**

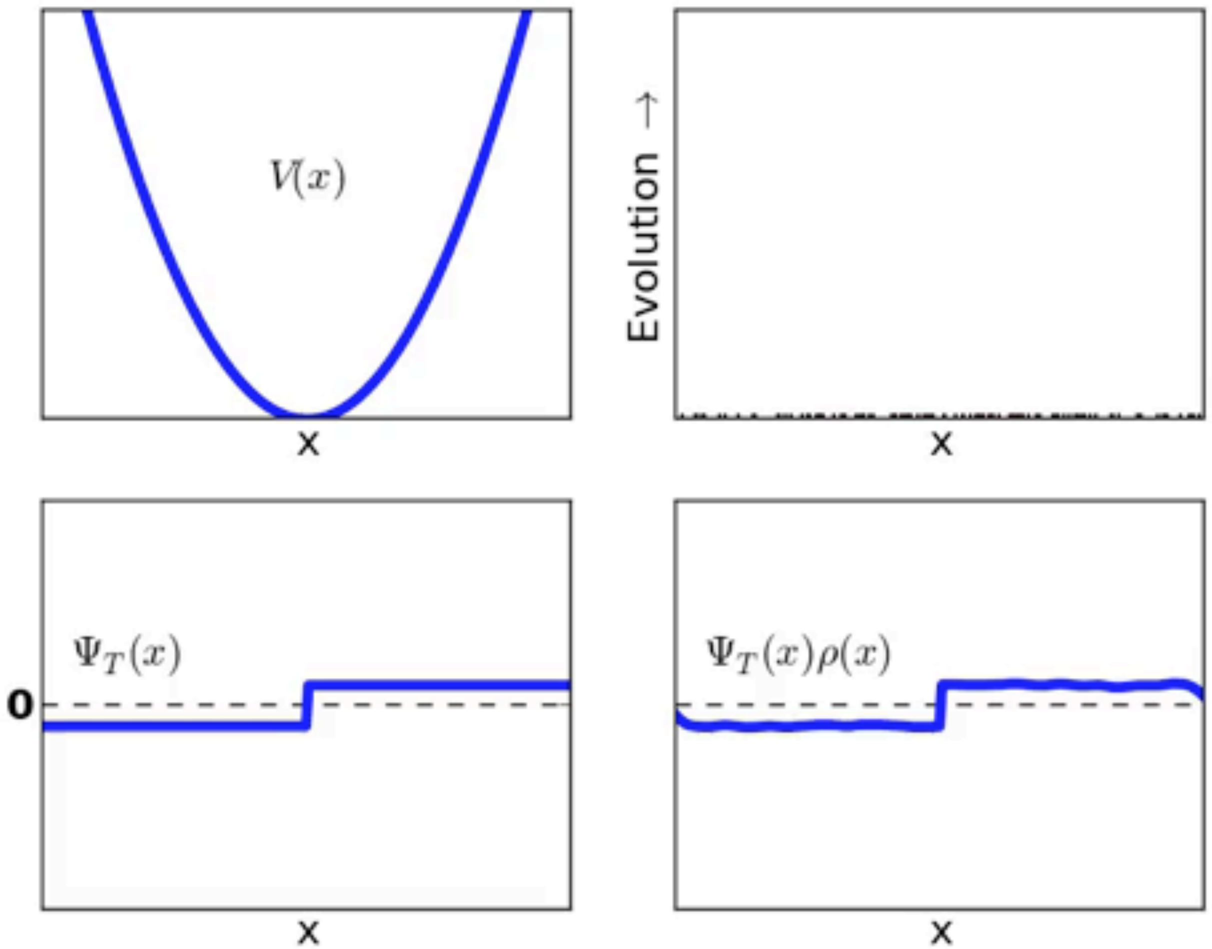
**Kinetic energy is diffusion, potential energy is birth/death.**

**Walkers are inherently positive**

**Obtains bosonic solution by default**

**Would like to force positive/ negative walkers for fermionic solution**






**Fixed node diffusion Monte Carlo**

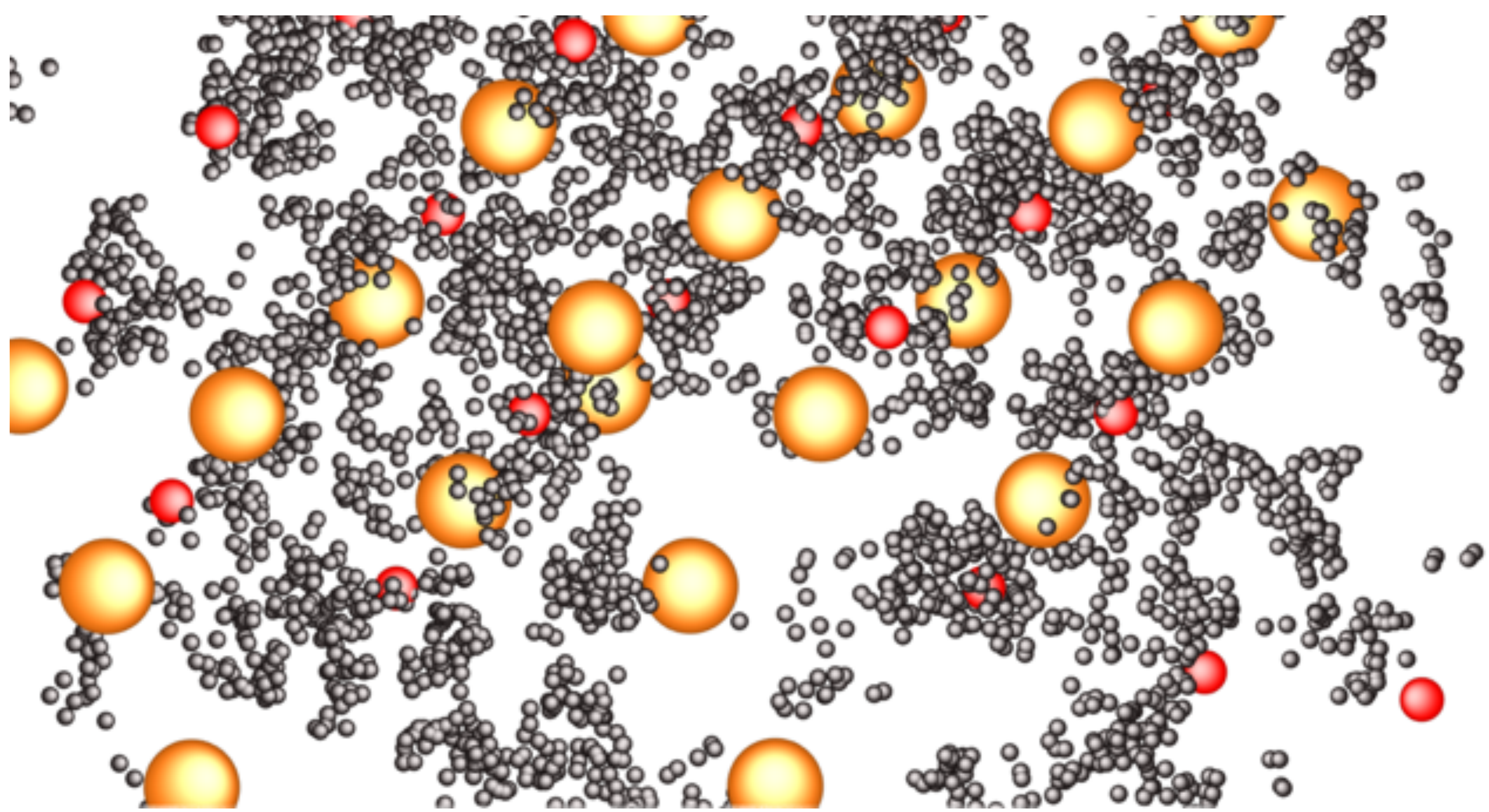
**Don't allow walkers to cross nodes.**

**Signs of walkers determined by trial function.**

**Allows for excited states and for fermions**

**Walkers move in $3N_e$-dimensional space**

**Trial function determined by fermionic wave function**



**Atomic positions, fundamental constants**

↓

Density functional theory

↓

Slater determinant

↓

Variational Monte Carlo

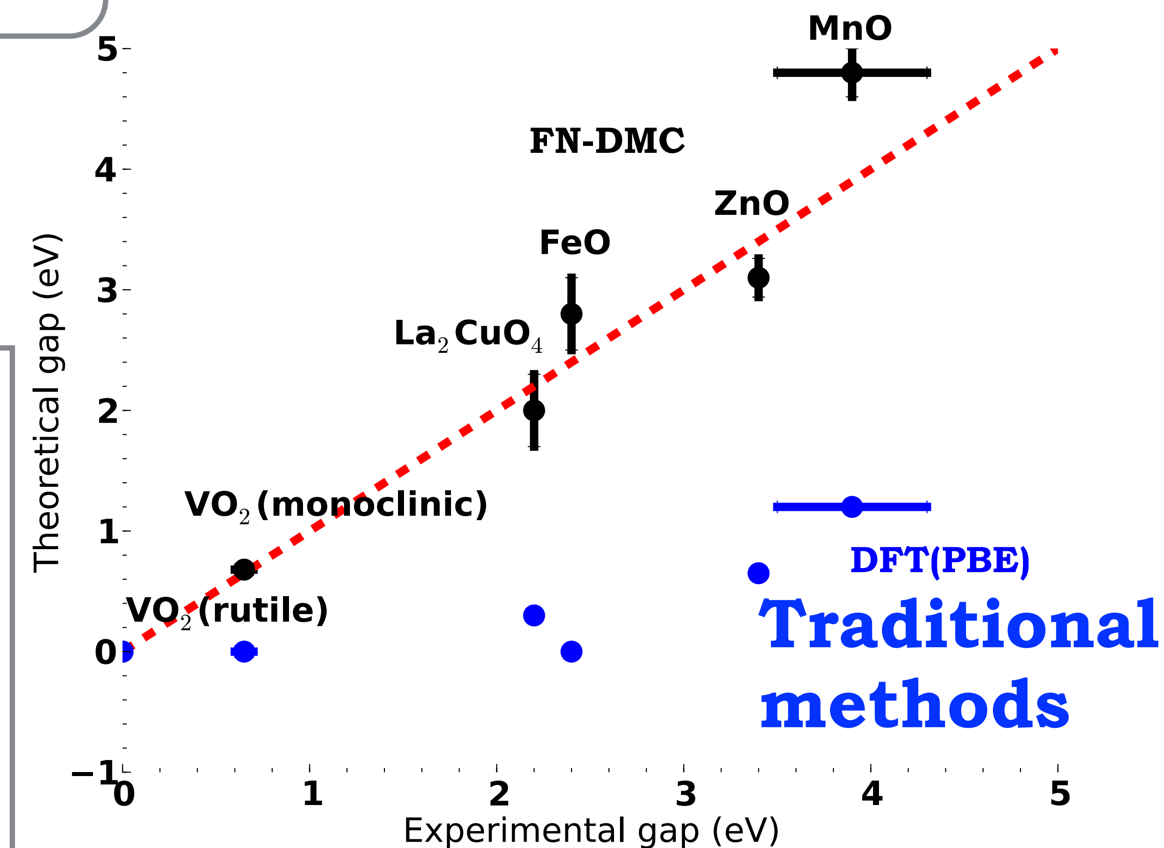
↓

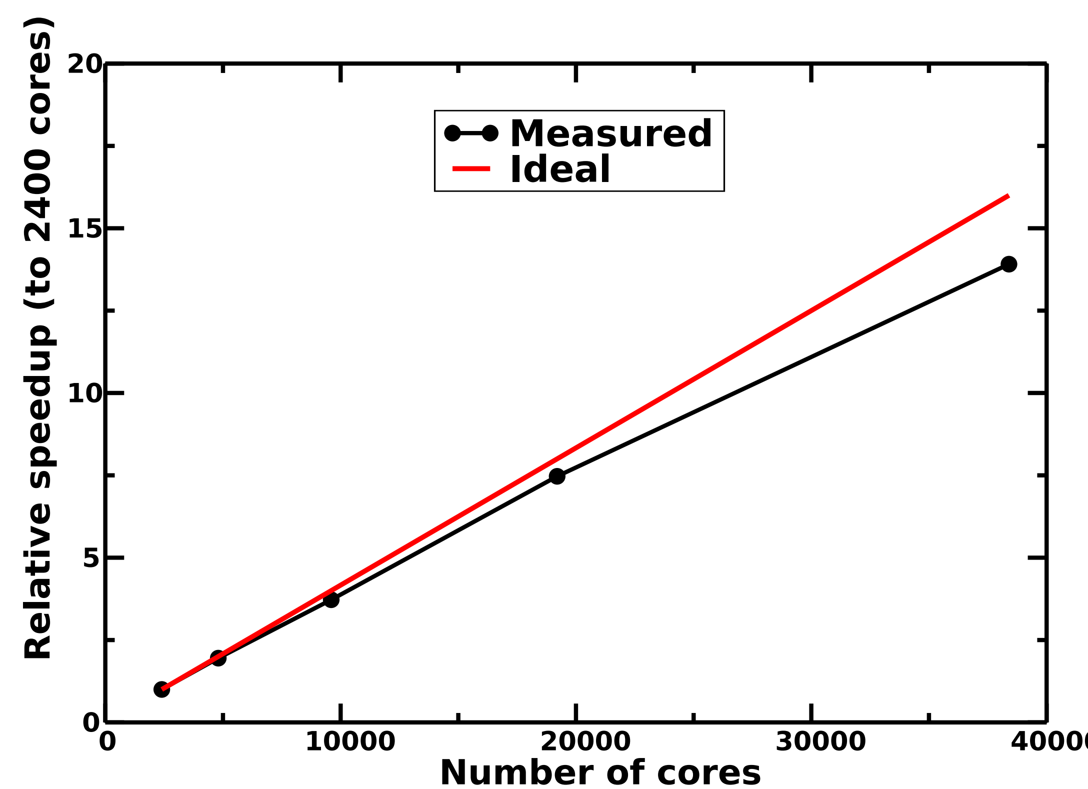
Slater-Jastrow

↓

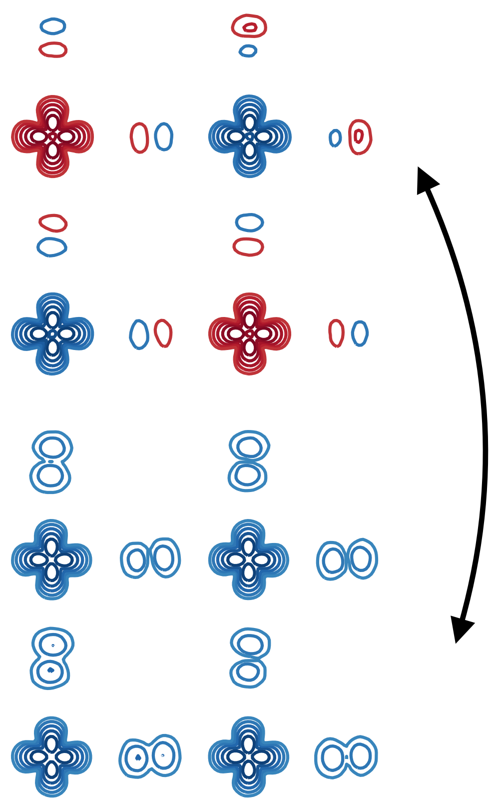
Fixed node diffusion Monte Carlo

**qwalk.org**



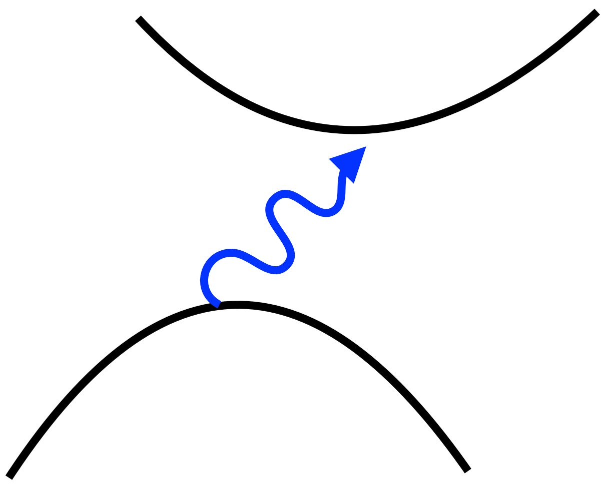



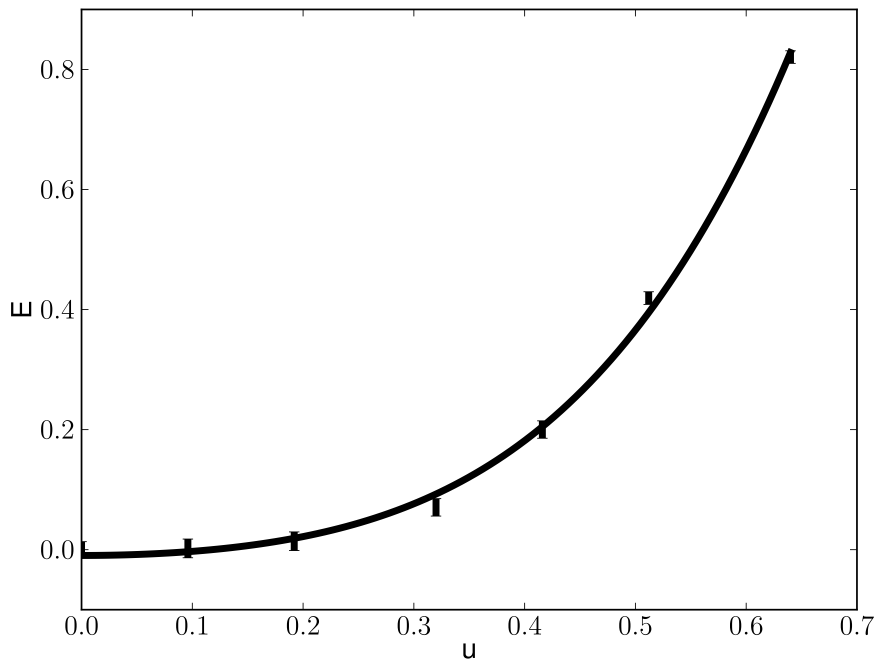
# How we calculate quantities on the cuprates



**Superexchange parameter J:**

**energy difference between AFM ordered and FM ordered spins**

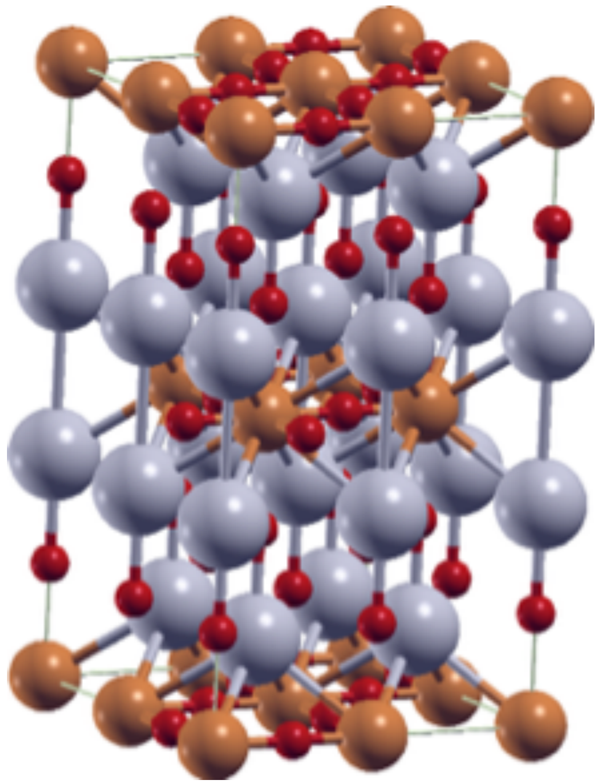


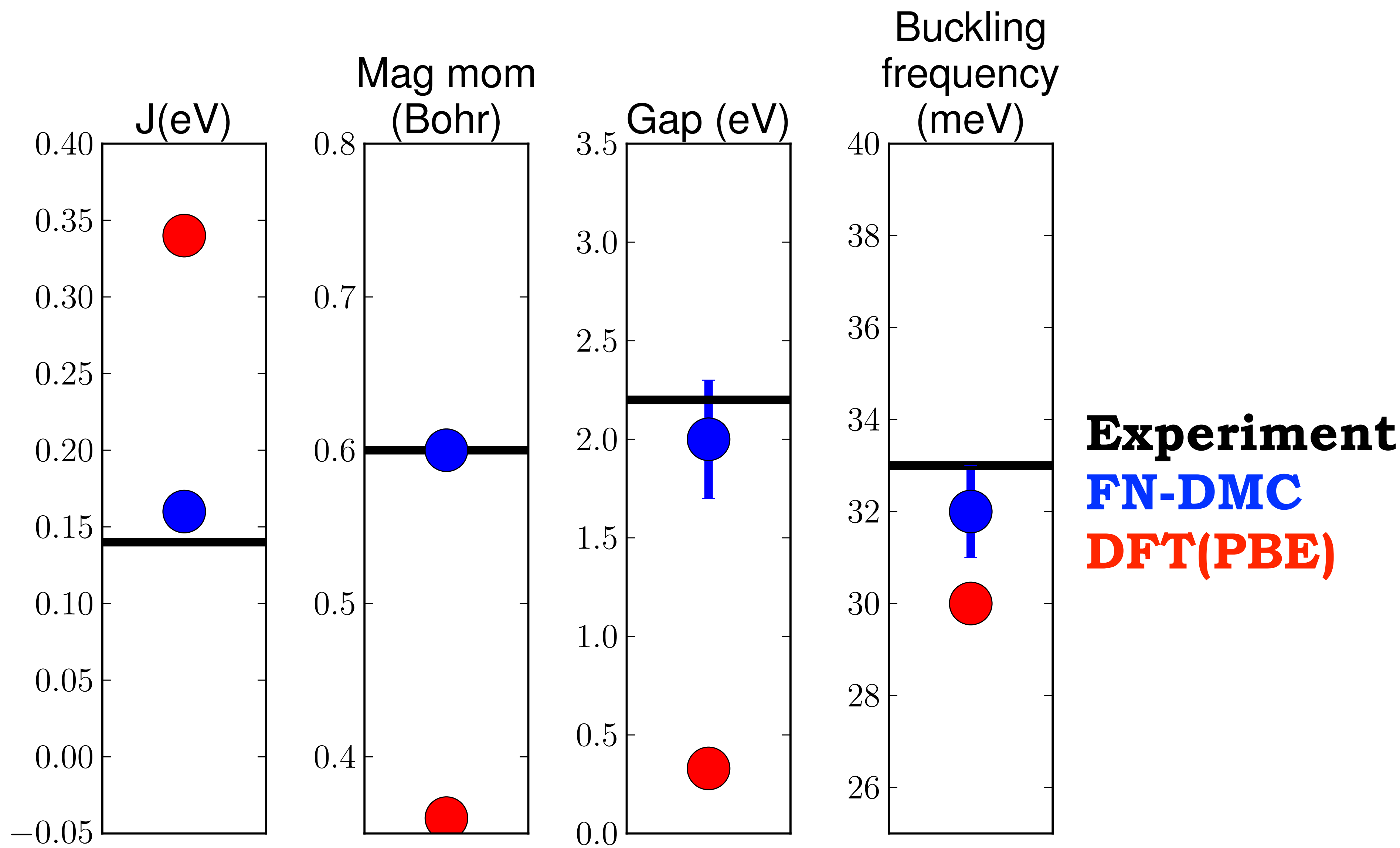



**Phonon frequency: calculate E(u), fit.**

**Gap: use excited state nodes**

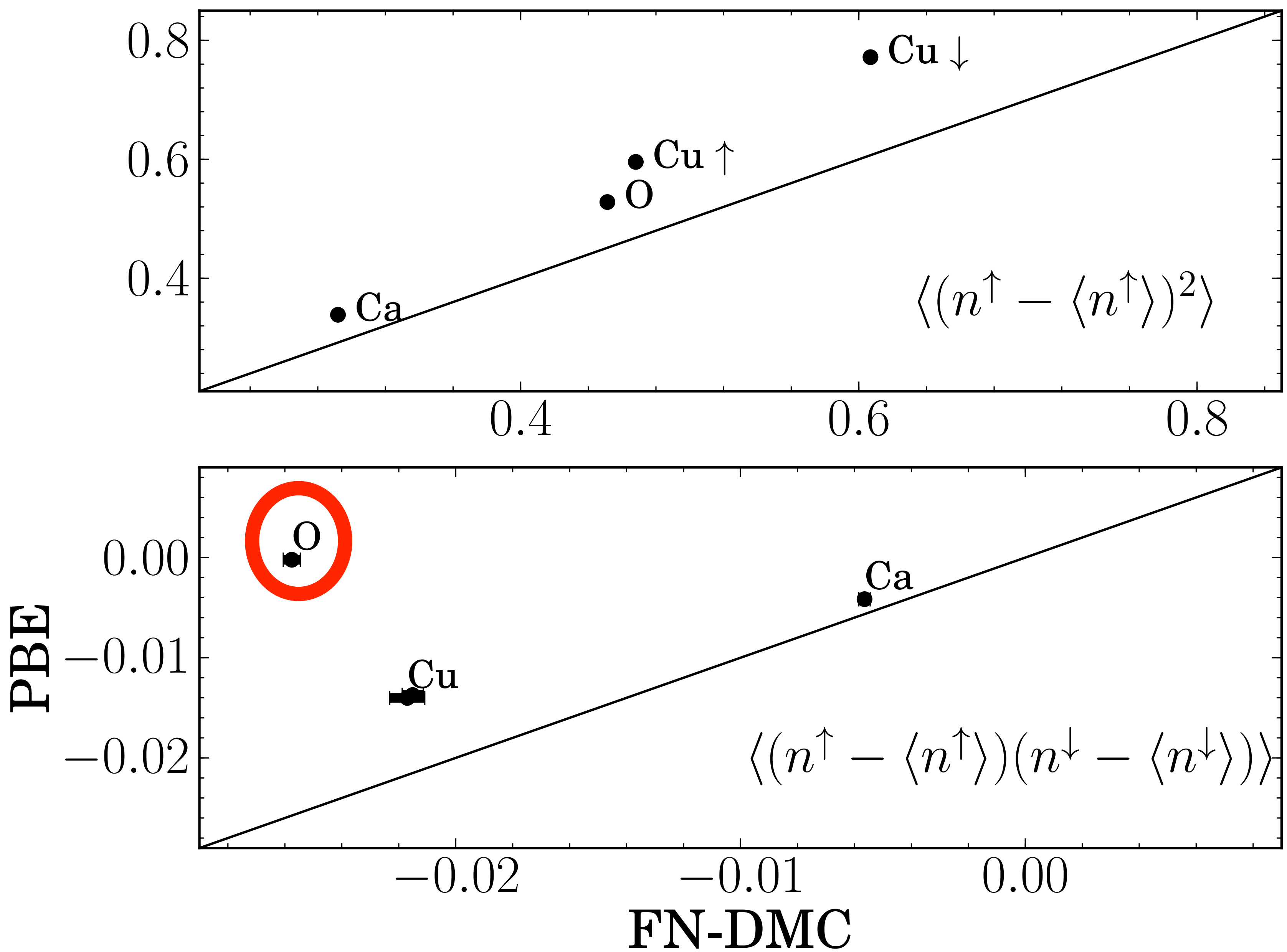
# High accuracy on high $T_c$






L.K. Wagner and P. Abbamonte arXiv:1402.4680

# What's wrong with density functional theory?




**How mobile electrons from a given atom are 't'**

**How much up/down electrons repel each other 'U'**

**Up/down in oxygen atoms are strongly correlated!**

# Origin of superconductivity

Charge carriers

Not strong enough

Isotope effects

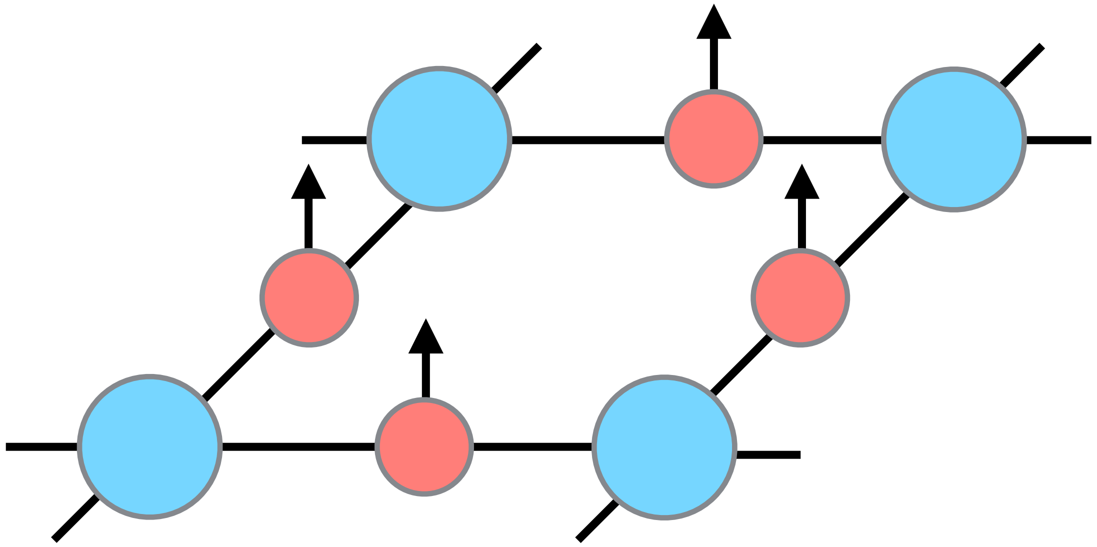
Phonons

Magnetism

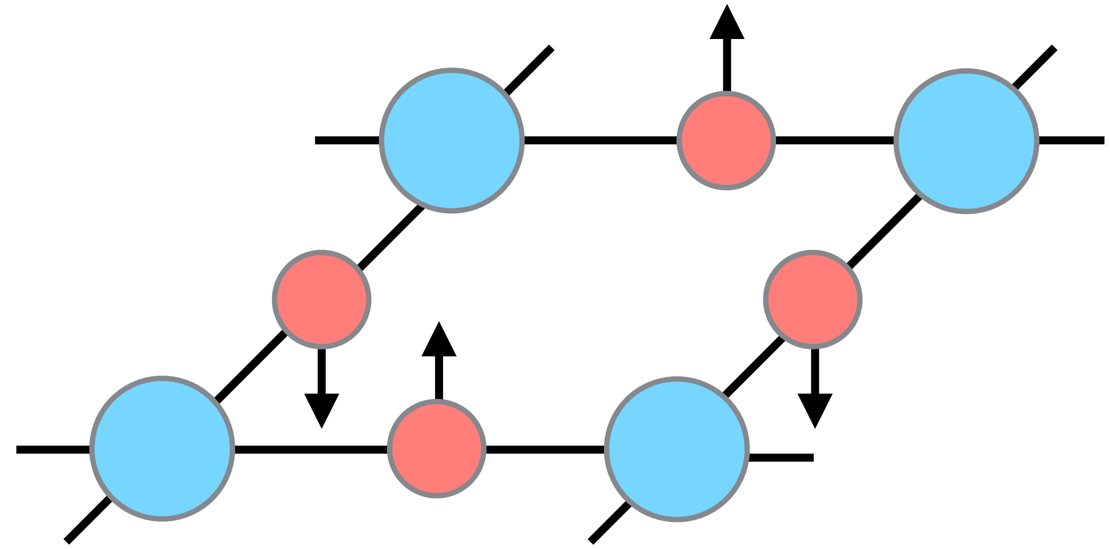
????

**What is the relationship between structure and spin?**

# Can spin-lattice coupling explain the experimental shifts?



$A_{1g}$



$B_{1g}$

**Does not shift on superconductivity**

**Shifts on superconductivity**

**Do they also change with magnetic state?**
**(computer experiment)**

**No!**

**Yes!**

**Blue Waters has allowed us to make progress on one of the most challenging questions in condensed matter physics: high temperature superconductivity.**

**We now have a technique that can solve the many-body Schroedinger equation to sufficient accuracy to make predictions.**

**Initial results have allowed us to verify experimental suspicions about the way particles interact in these systems.**


**Thanks to:**

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