Stabilizing Room-Temperature Superconductivity in Hydrides by Nonequilibrium Driving

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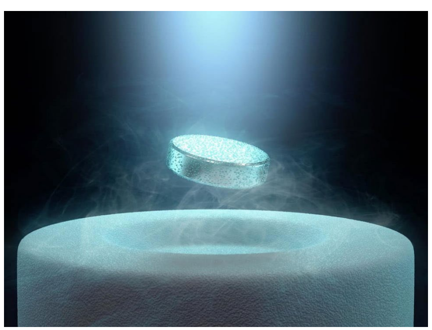
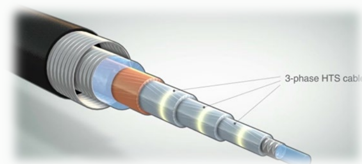
Superconductivity

- **Most important quantum phases**
  - Non-resistance
  - Diamagnetism

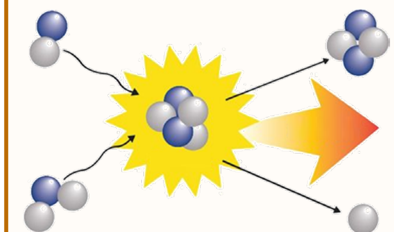
- **Broad applications**
  - Dissipation-less power transmission
  - Quantum computing (qubits)
  - Controlled nuclear fusion
  - Public transportation

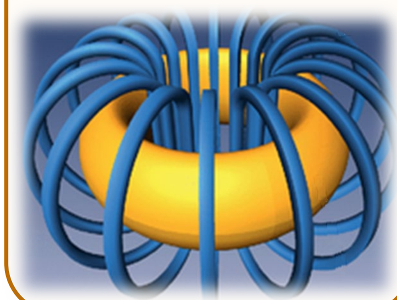


Power transmission

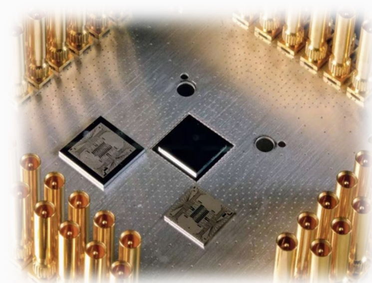


Controlled fusion





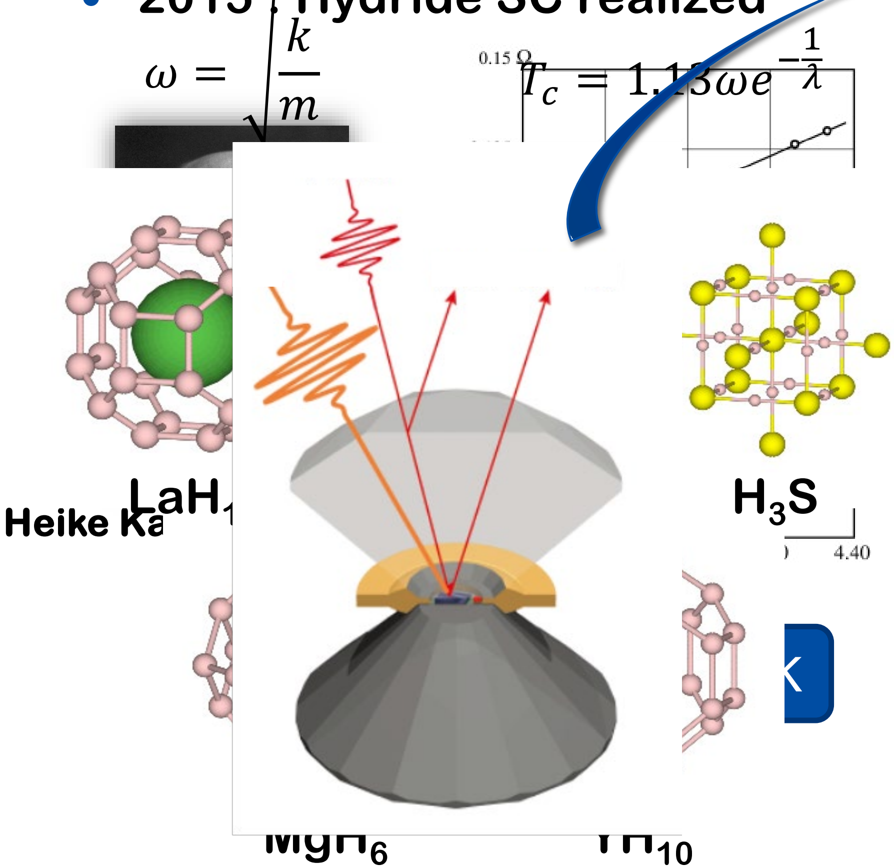
Quantum computing

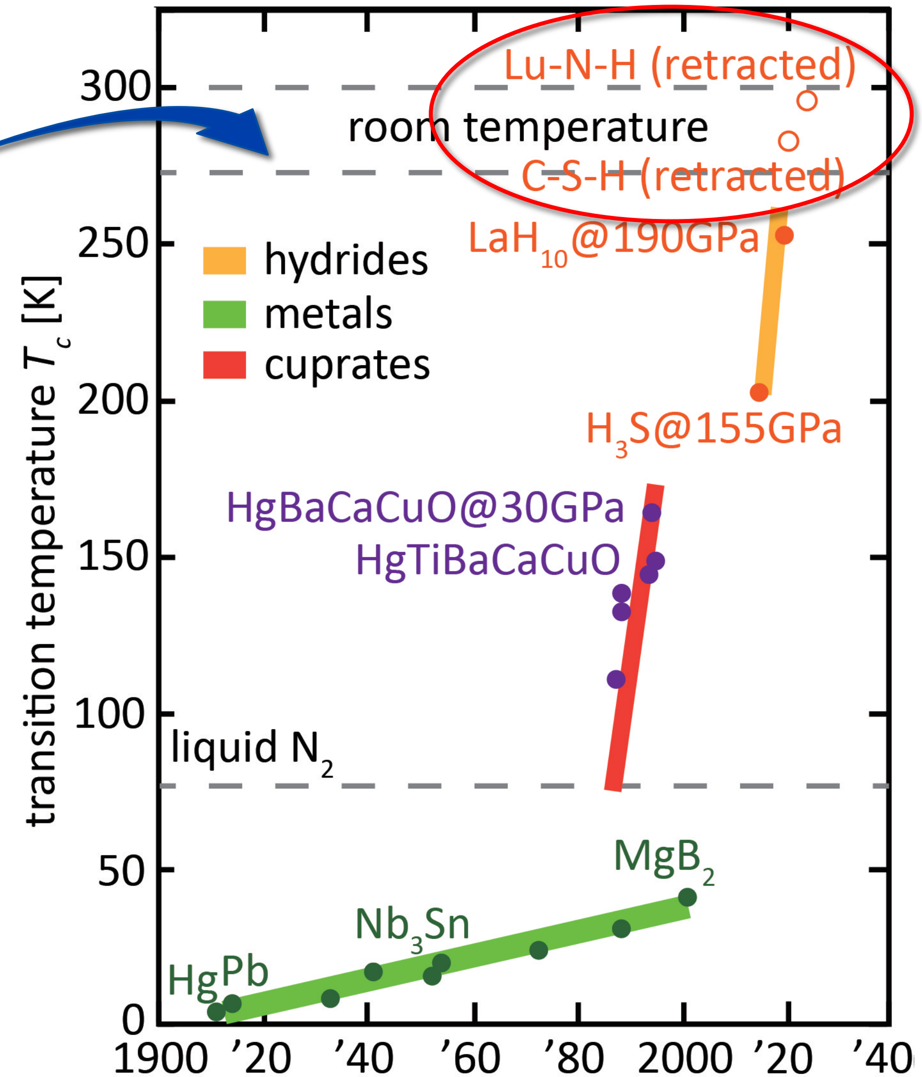


Transportation

Roadmap of Superconductors

- **1911 : Superconductivity (SC) first observed in Hg**
- **1957 : BCS theory**
- **1986 : Cuprate superconductors**
- **2015 : Hydride SC realized**





Equilibrium Band Structure of LaH_{10}

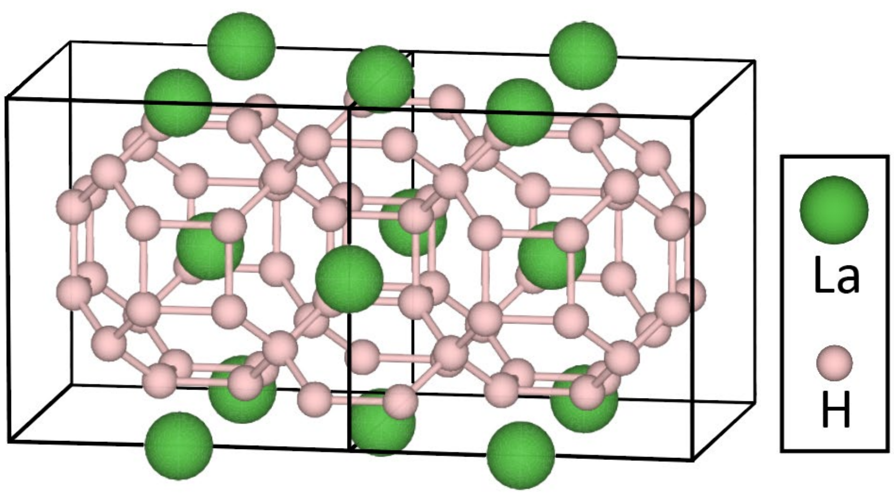
- **First principles calculation**
  - Density functional theory (DFT) calculation
  - Wannier tight-binding model simulation
    - Band Structure Benchmark
    - Equilibrium DOS calculation

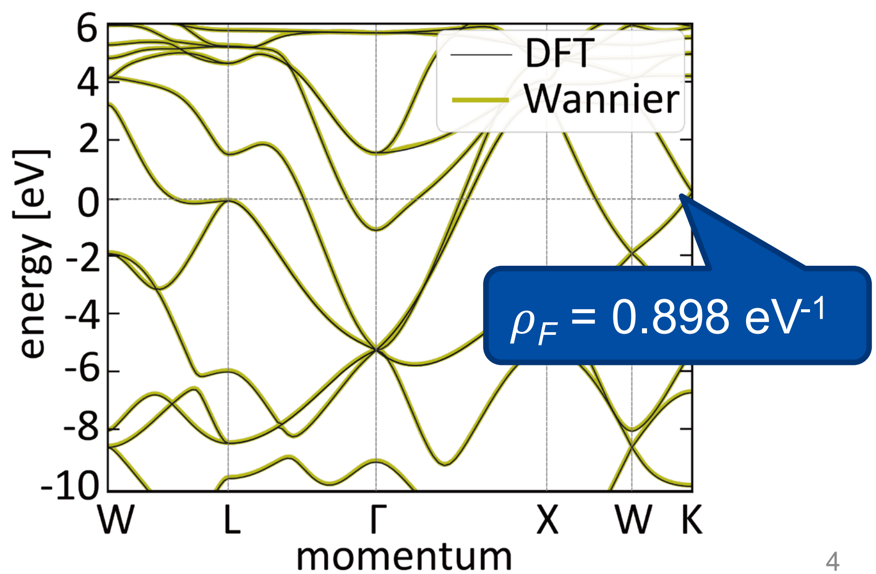
QUANTUMESPRESSO

WANNIER90

$$\mathcal{H} = \sum_{\substack{jl \\ \alpha\beta\sigma}} H_{jl}^{(\alpha\beta)} c_{l\beta\sigma}^{\dagger} c_{j\alpha\sigma} = \sum_{\substack{j \\ \alpha\sigma}} E_{\alpha} c_{j\alpha\sigma}^{\dagger} c_{j\alpha\sigma} + \sum_{\substack{jl \\ \alpha\beta\sigma}} t_{jl}^{(\alpha\beta)} (c_{l\beta\sigma}^{\dagger} c_{j\alpha\sigma} + h.c.)$$

Site energy term — Hopping energy term



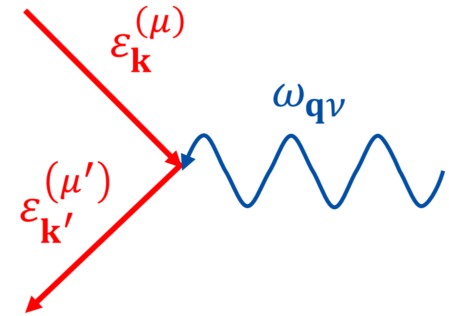


[1] Giannozzi *et al*. *J. Phys.: Condens. Matter* **29**, 465901 (2017)
[2] Pizzi *et al*. *J. Phys.: Condens. Matter* **32**, 165902 (2020)

Electron-Phonon Coupling Calculations

- **Electron-phonon coupling for superconductivity**
  - DFPT phonon and el-ph coupling matrix elements

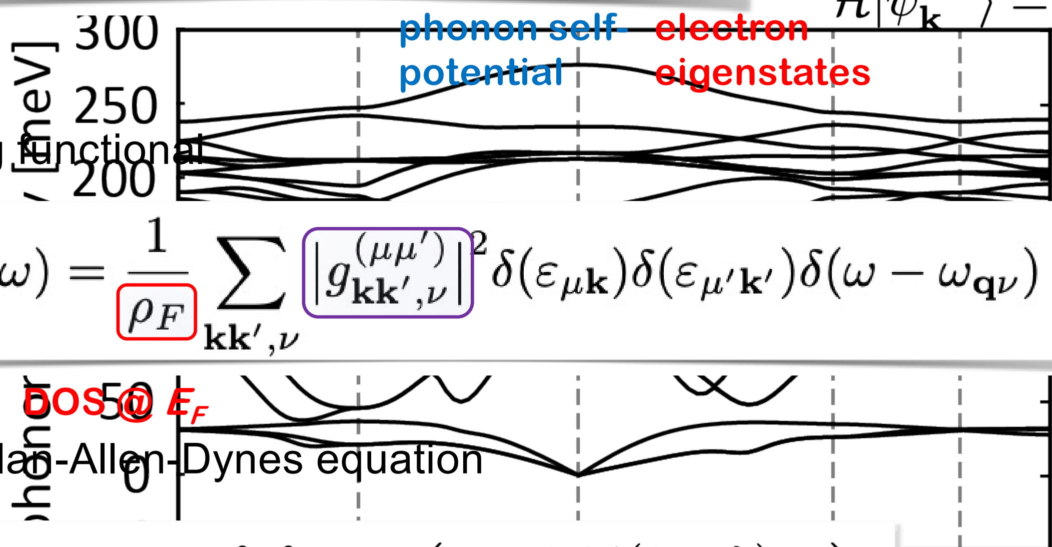
$$g_{\mathbf{k}\mathbf{k}',\nu}^{(\mu\mu')} = \sqrt{\frac{\hbar}{2m_0\omega_{\mathbf{q}\nu}}}\langle\psi_{\mathbf{k}'}^{(\mu')}|\partial_{\mathbf{q}\nu}V|\psi_{\mathbf{k}}^{(\mu)}\rangle$$



$$\mathcal{H}|\psi_{\mathbf{k}}^{(\mu)}\rangle = E_{\mathbf{k}}^{(\mu)}|\psi_{\mathbf{k}}^{(\mu)}\rangle$$

phonon self-potential

electron eigenstates



  - Eliashberg functional

$$\alpha^2F(\omega) = \frac{1}{\rho_F}\sum_{\mathbf{k}\mathbf{k}',\nu}\left|g_{\mathbf{k}\mathbf{k}',\nu}^{(\mu\mu')}\right|^2\delta(\varepsilon_{\mu\mathbf{k}})\delta(\varepsilon_{\mu'\mathbf{k}'})\delta(\omega-\omega_{\mathbf{q}\nu})$$

DOS @ E_F

  - Full McMillan-Allen-Dynes equation

$$T_c = \omega_{\log}\frac{f_1f_2}{1.2}\exp\left(\frac{-1.04(1+\lambda)}{\lambda-\mu^*(1+0.62\lambda)}\right)$$

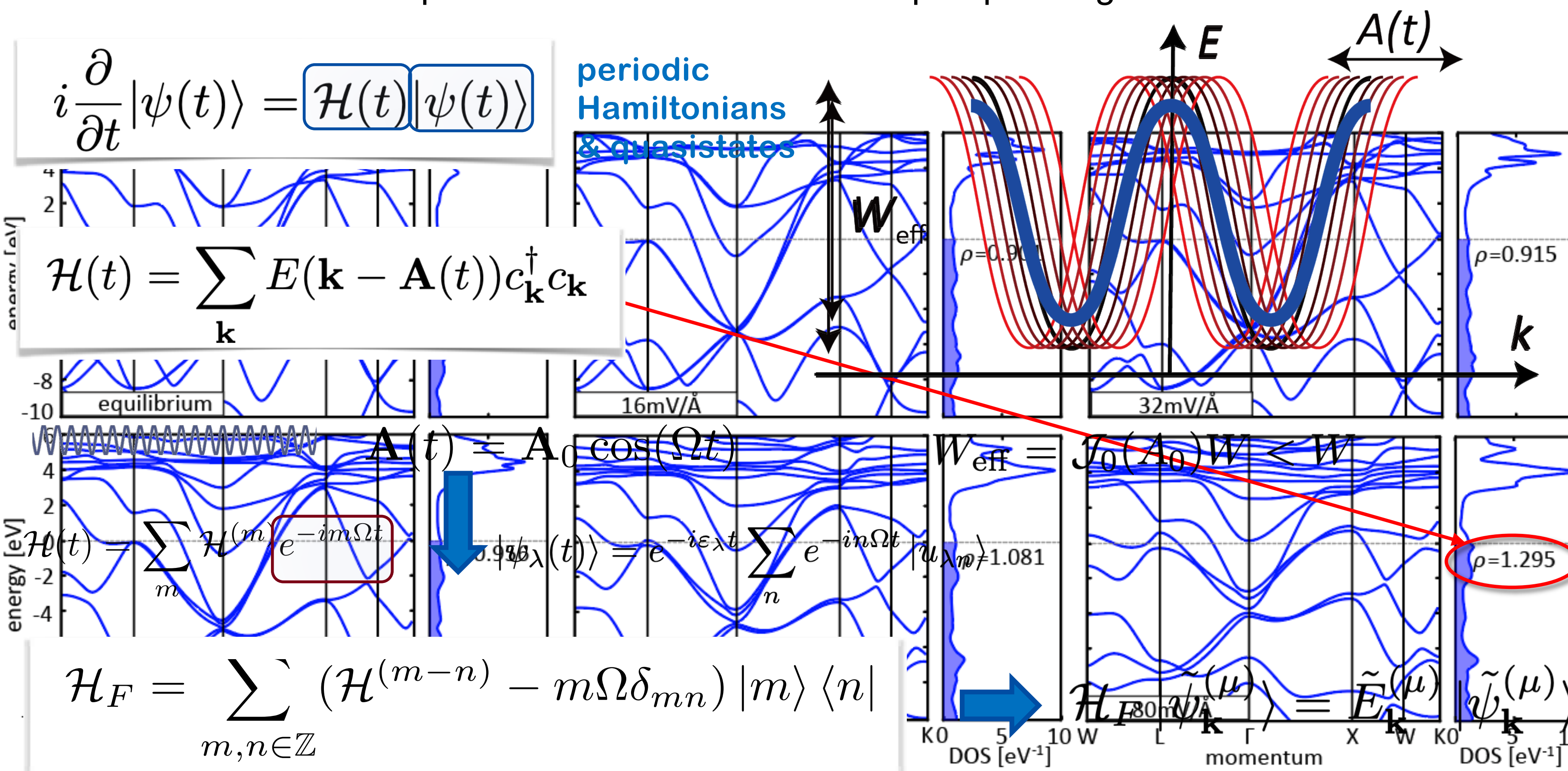
$$\lambda = \int_0^\infty \frac{2}{\omega}\alpha^2F(\omega)d\omega$$

Our T_c: 258 K, accepted T_c: 265 K[2]

[1] Lee *et al*. *npj Comput. Mater.* **9**, 156 (2023)
[2] Wang *et al*. *Phys. Rev. B* **100**, 060502(R) (2023)

Nonequilibrium Band Evolution of LaH_{10}

- **Nonequilibrium electron structures of LaH_{10}**
  - Approximations for time-dependent Hamiltonian
  - Diagonalize Floquet Hamiltonians $\mathcal{H}_F$ for band structure
  - Evolution of nonequilibrium DOS under different pump strengths



Nonequilibrium Electron-Phonon Coupling of LaH_{10}

- **Electron-phonon coupling and T_c calculations**
  - Nonequilibrium el-ph coupling matrix elements $\tilde{g}$
  - Nonequilibrium Eliashberg functional $\alpha^2\tilde{F}(\omega)$
  - El-ph coupling strength $\tilde{\lambda}$ & transition temperature T_c

phonon dynamical matrices

equilibrium system

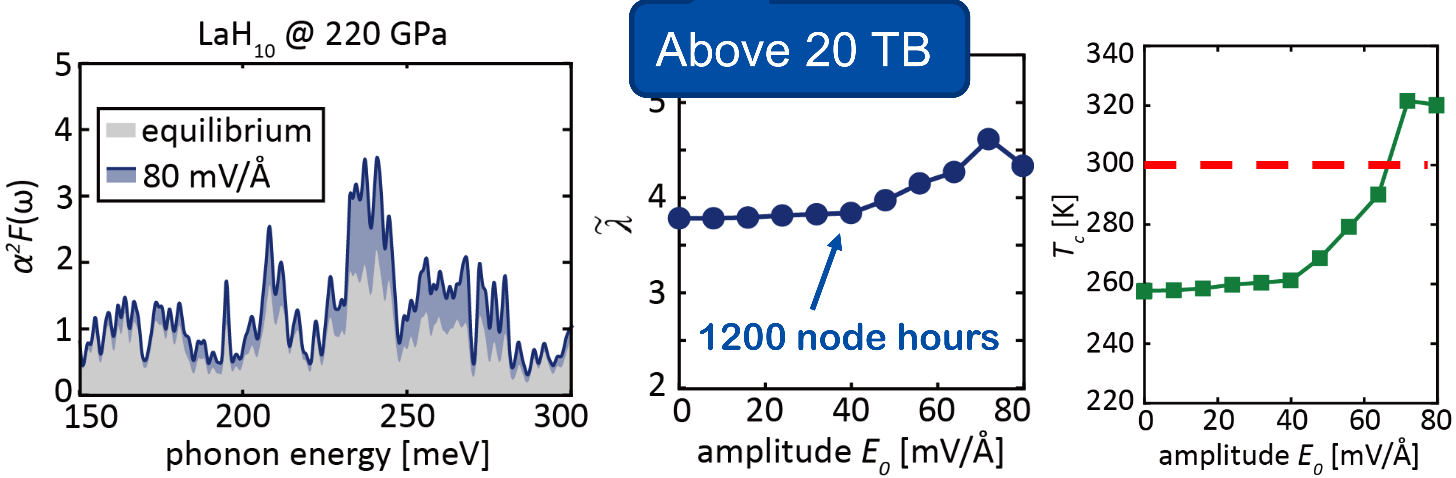
$$\mathcal{H}|\psi_{\mathbf{k}}^{(\mu)}\rangle = E_{\mathbf{k}}^{(\mu)}|\psi_{\mathbf{k}}^{(\mu)}\rangle \;\Rightarrow\; g_{\mathbf{kk}',\nu}^{(\mu\mu')} = \sqrt{\frac{\hbar}{2m_0\omega_{\mathbf{q}\nu}}}\langle\psi_{\mathbf{k}'}^{(\mu')}|\partial_{\mathbf{q}\nu}V|\psi_{\mathbf{k}}^{(\mu)}\rangle$$

nonequilibrium steady-state system (Floquet)

$$\mathcal{H}_F|\tilde{\psi}_{\mathbf{k}}^{(\mu)}\rangle = \tilde{E}_{\mathbf{k}}^{(\mu)}|\tilde{\psi}_{\mathbf{k}}^{(\mu)}\rangle \;\Rightarrow\; \tilde{g}_{\mathbf{kk}',\nu}^{(\mu\mu')} = \sqrt{\frac{\hbar}{2m_0\omega_{\mathbf{q}\nu}}}\langle\tilde{\psi}_{\mathbf{k}'}^{(\mu')}|\partial_{\mathbf{q}\nu}V|\tilde{\psi}_{\mathbf{k}}^{(\mu)}\rangle$$

electron eigenstates

Above 20 TB



room temperature

Total cost: 40,000–50,000 node hours

Xie *et al*. arXiv: 2312.12706, under review of *Nature Communications* (2024).

Summary

A dynamic approach to increase T_c in hydrides

- Light-induced room temperature superconductivity
- Elevated DOS and electron-phonon coupling contribute to T_c increase
- Pressure dependence & polarization analysis (not shown in presentation)

Acknowledgements

- **Collaborators**
  - Dr. Wei-Chih Chen @ Clemson University
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- **Computation Resources**
  - Frontera LRAC: DMR21001

    Electron-Phonon Coupling in Correlated Quantum Materials

Thanks for your attention!