SIMONS FOUNDATION

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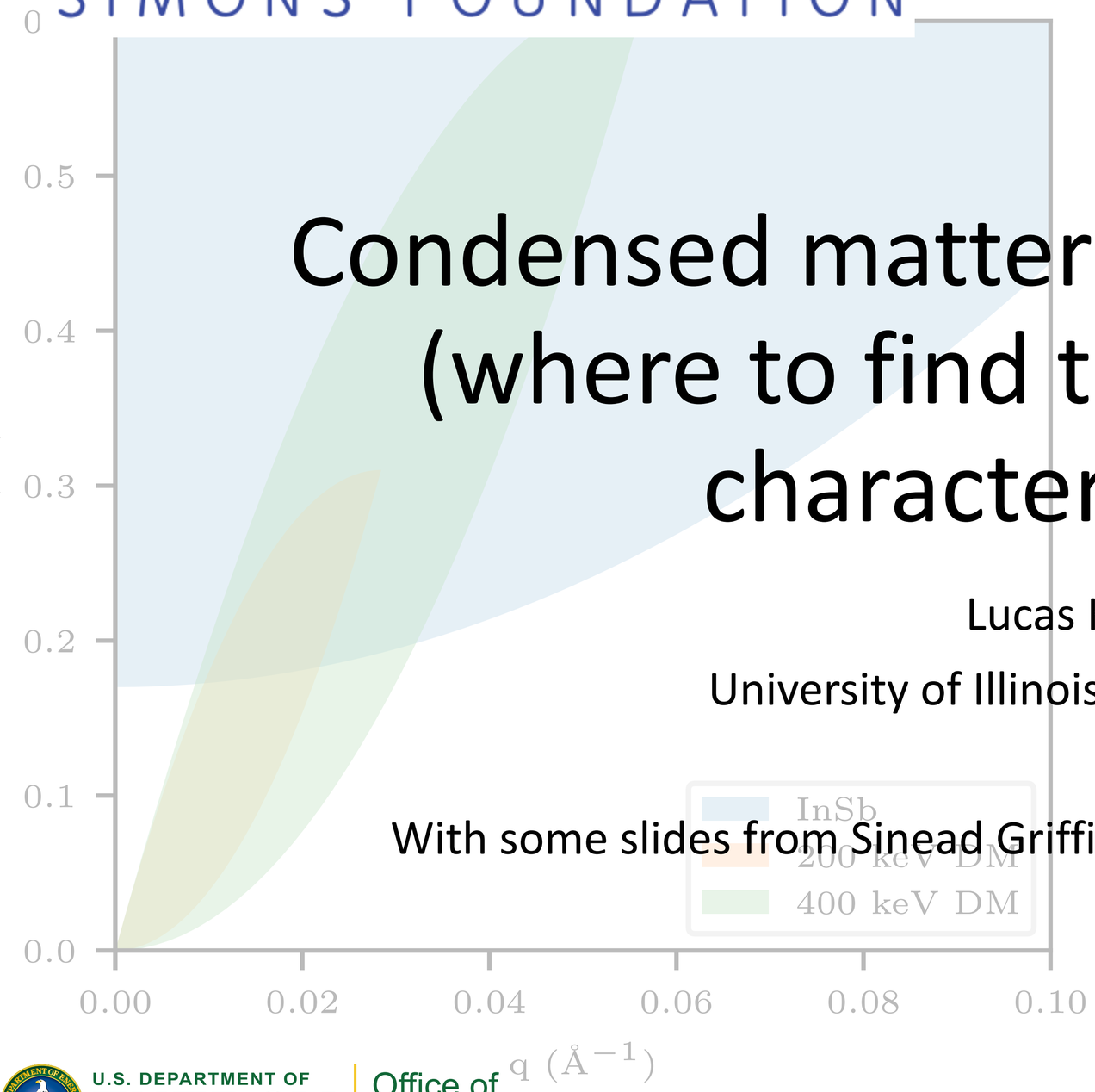

Condensed matter systems of interest (where to find them and how to characterize them)

Lucas K. Wagner

University of Illinois at Urbana-Champaign

With some slides from Sinead Griffin (LBNL) and Peter Abbamonte (UIUC)

U.S. DEPARTMENT OF ENERGY | Office of Science

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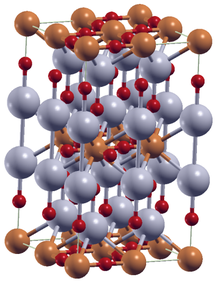
A bit about me



+

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

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

minimal approximations including electron correlations explicitly

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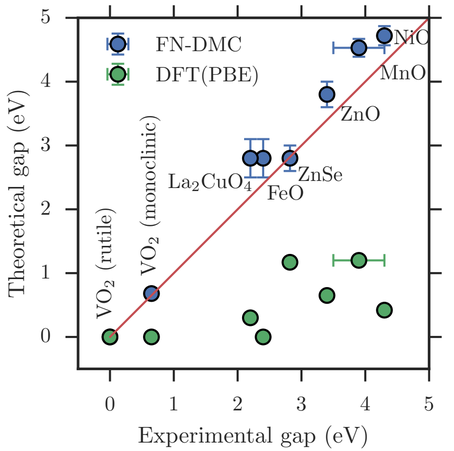
First principles quantum Monte Carlo

Obtain the ground state wave function by projection

$$\frac{\left\langle \Psi_T \left| e^{-\tau H} \mathcal{O} e^{-\tau H} \right| \Psi_T \right\rangle}{\left\langle \Psi_T \left| e^{-\tau H} e^{-\tau H} \right| \Psi_T \right\rangle}$$



$$H = -\frac{1}{2}\nabla^2 + \sum_{ij}\frac{1}{r_{ij}} + \ldots$$

Use resolution of identity

$$\left\langle \Psi_T \left| e^{-\tau H} \mathcal{O} e^{-\tau H} \right| \Psi_T \right\rangle = \int \langle \Psi_T | R_1 \rangle \langle R_2 | e^{-\tau H} | R_3 \rangle \langle R_3 | \mathcal{O} | R_4 \rangle \langle R_4 | e^{-\tau H} | R_5 \rangle \langle R_5 | \Psi_T \rangle dR_1 dR_2 dR_3 dR_4 dR_5$$

Each R is a many-body coordinate. This is a 15N dimensional integral. Evaluate using Monte Carlo.

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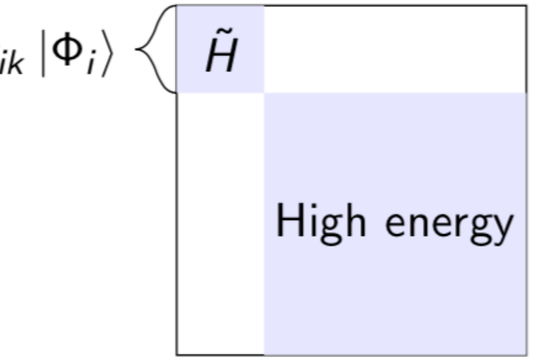
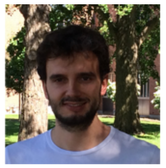
Some things my group does

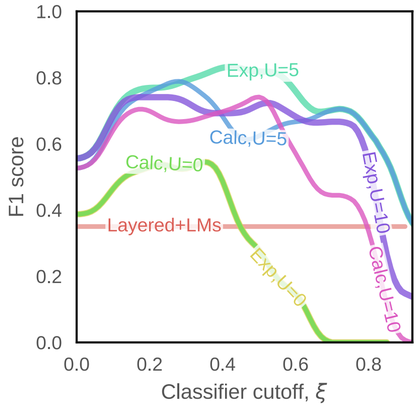




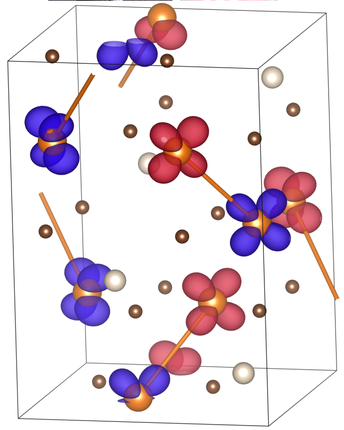
Interacting effective Hamiltonians

10.3389/fphy.2018.00043

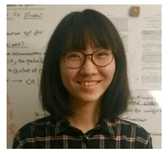



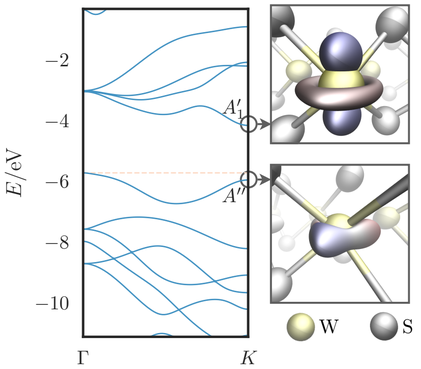


Attempting to predict and understand unconventional superconductivity

Computing magnetic properties of materials



Spin-orbit coupling with explicit electronic interactions
arXiv: 1809.04133

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Part 1: New (old) materials that could be useful for dark matter detection

Part 2: Condensed matter experiment and computation to understand detection limits better for a known material.

“Materials by design”

193,000 inorganic crystals (some duplicates)

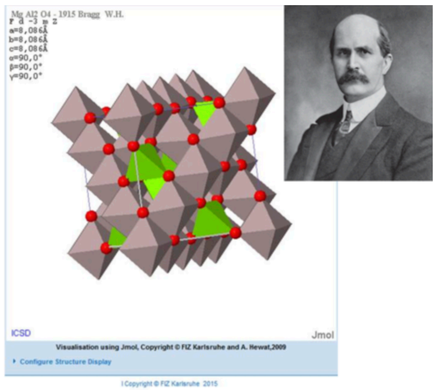
ICSD – the Inorganic Crystal Structure Database

The Information Service for Inorganic Crystal Structures

ICSD is the world's largest database for fully identified inorganic crystal structures. It is produced by FIZ Karlsruhe and currently contains about 193,000 crystal structures. Updates are made twice a year (in spring and in fall) with data taken from scientific journals and other sources.

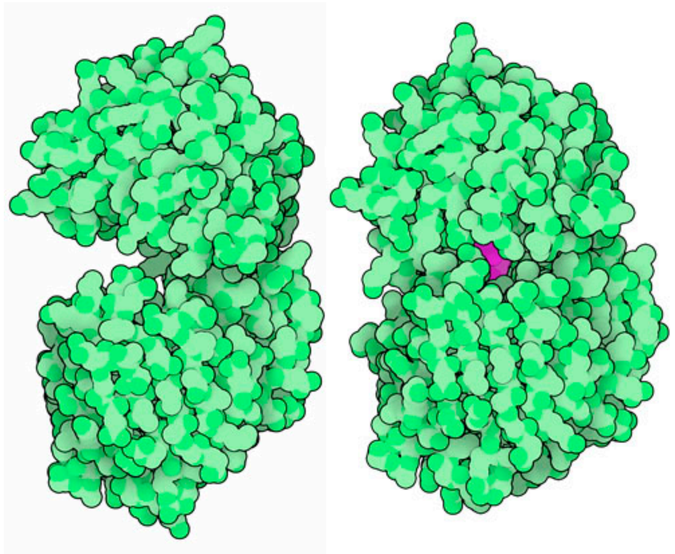
Thanks to these many heterogeneous data sources the database has a wide coverage. ICSD is also updated retroactively. As all steps of the value generation chain – looking for sources, database production, data management – are performed here at FIZ Karlsruhe, we can always meet and maintain our high standards as to the reliability of the data.

About 4,000 structures are added to ICSD each year. The oldest records date back to the year 1913 and contain information from publications by William Henry Bragg and his son.



William Henry Bragg with one of the crystal structures he identified

Protein data bank: 42,000 distinct protein sequences



391,334 organic and inorganic crystals (some duplicates)

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Many known materials that could (in principle) detect very light DM

Gap(eV)

IV-VI	3	Lead tin telluride	$Pb_{1-x}Sn_xTe$	0-0.29		Used in infrared detectors and for thermal imaging
IV	1	Gray tin, *α*-Sn	Sn	0.00,[7] 0.08[8]	indirect	Low temperature allotrope (diamond cubic lattice).
II-V	2	Cadmium arsenide	Cd_3As_2	0.14		N-type intrinsic semiconductor. Very high electron mobility. Used in infrared detectors, photodetectors, dynamic thin-film pressure sensors, and magnetoresistors. Recent measurements suggest that 3D Cd_3As_2 is actually a zero band-gap Dirac semimetal in which electrons behave relativistically as in graphene.[15]
III-V	2	Indium antimonide	InSb	0.17[4]	direct	Used in infrared detectors and thermal imaging sensors, high quantum efficiency, low stability, require cooling, used in military long-range thermal imager systems. AlInSb-InSb-AlInSb structure used as quantum well. Very high electron mobility, electron velocity and ballistic length. Transistors can operate below 0.5V and above 200 GHz. Terahertz frequencies maybe achievable.
IV-VI	2	Tin telluride	SnTe	0.18		Complex band structure.
IV-VI	2	Lead selenide	PbSe	0.27	direct	Used in infrared detectors for thermal imaging. Nanocrystals usable as quantum dots. Good high temperature thermoelectric material.
IV-VI	2	Lead telluride	PbTe	0.32		Low thermal conductivity, good thermoelectric material at elevated temperature for thermoelectric generators.
VI	1	Tellurium	Te	0.33		
III-V	2	Indium arsenide	InAs	0.36[4]	direct	Used for infrared detectors for 1–3.8 μm, cooled or uncooled. High electron mobility. InAs dots in InGaAs matrix can serve as quantum dots. Quantum dots may be formed from a monolayer of InAs on InP or GaAs. Strong photo-Dember emitter, used as a terahertz radiation source.
IV-VI	2	Lead(II) sulfide	PbS	0.37		Mineral galena, first semiconductor in practical use, used in cat's whisker detectors; the detectors are slow due to high dielectric constant of PbS. Oldest material used in infrared detectors. At room temperature can detect SWIR, longer wavelengths require cooling.
IV	1	Germanium	Ge	0.67[4][5]	indirect	Used in early radar detection diodes and first transistors; requires lower purity than silicon. A substrate for high-efficiency multijunction photovoltaic cells. Very similar lattice constant to gallium arsenide. High-purity crystals used for gamma spectroscopy. May grow whiskers, which impair reliability of some devices.
III-V	2	Indium nitride	InN	0.7[4]	direct	Possible use in solar cells, but p-type doping difficult. Used frequently as alloys.
V-VI	2	monoclinic Vanadium(IV) oxide	VO_2	0.7[20]	optical	stable below 67°C

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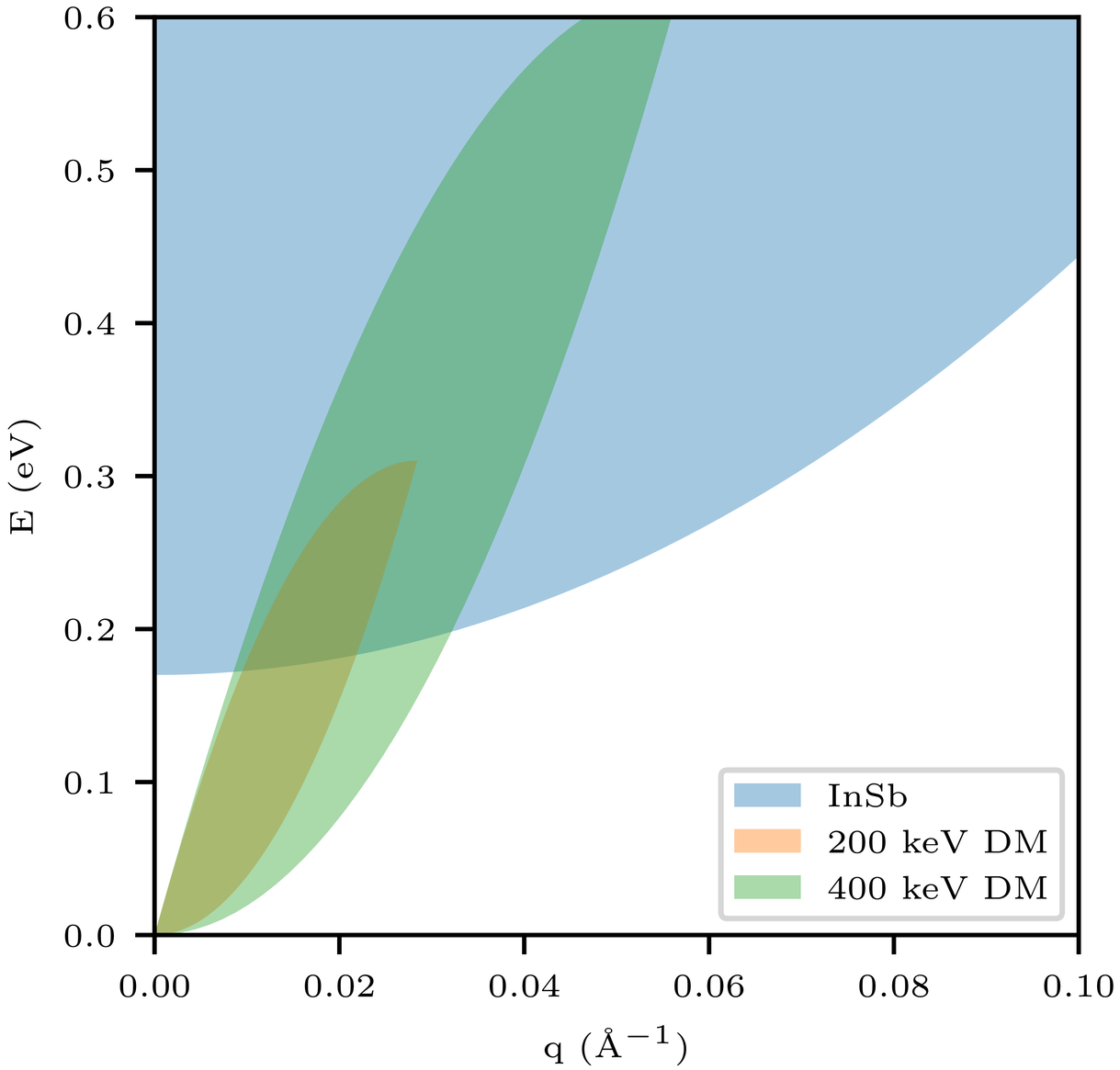
InSb: kinematic constraints for very light DM



Could extend reach (except radioactive In)

q dependence becomes important; many low-gap materials have light excitations -> no overlap

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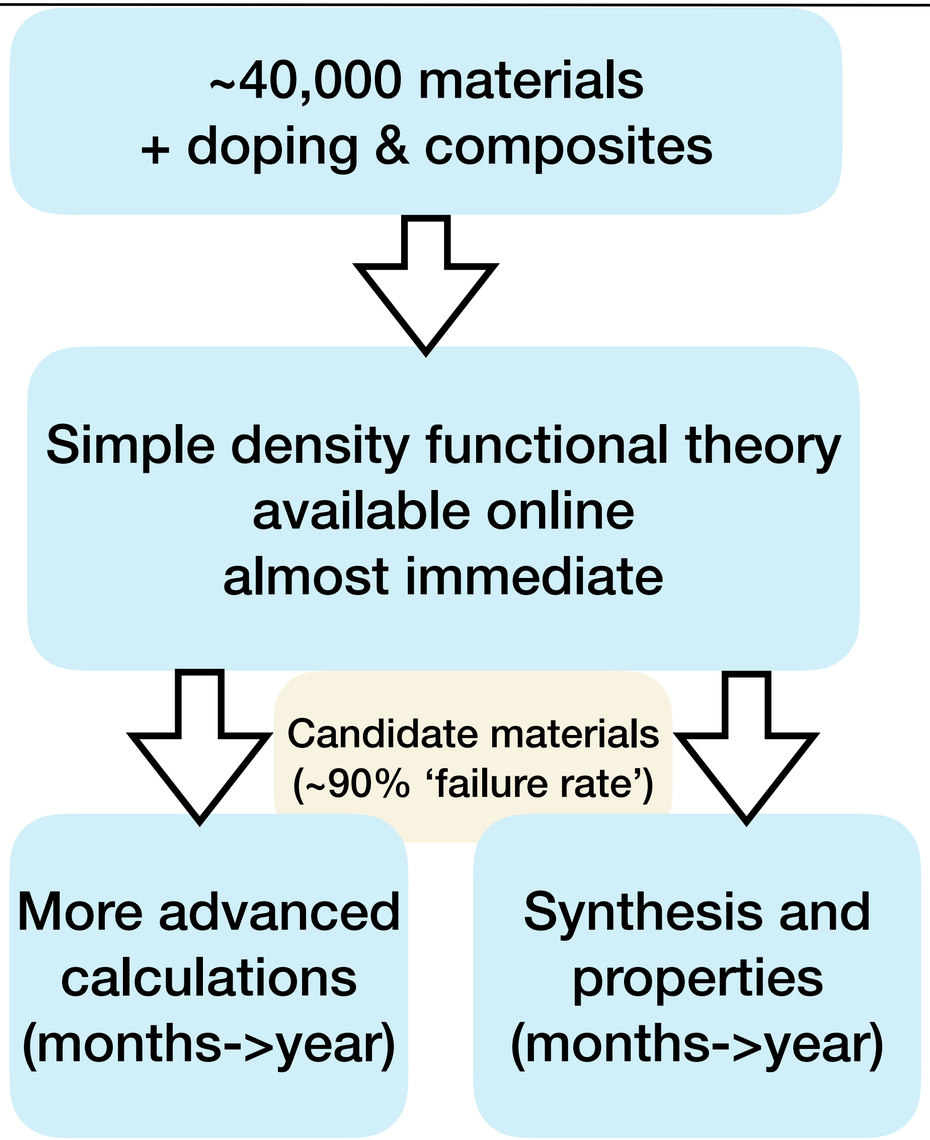
Materials by design



‘Failure rate’ comes from the material being impossible to synthesize, or the property filter of DFT not being accurate enough. We usually generate a ranked list.

After this we have a pretty good handle on how the material behaves and whether it .

Development to a working device can take years or decades after this, with substantial investment of capital.

People are trying to make this better.

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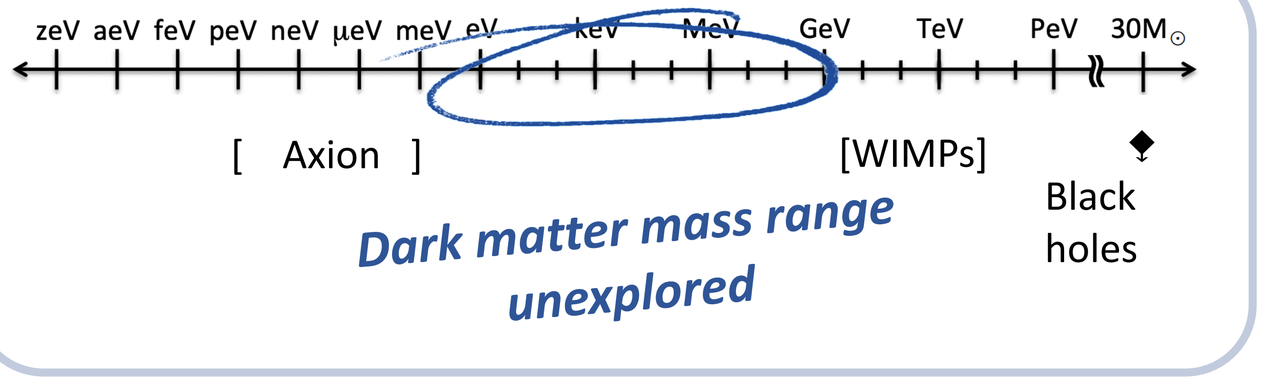
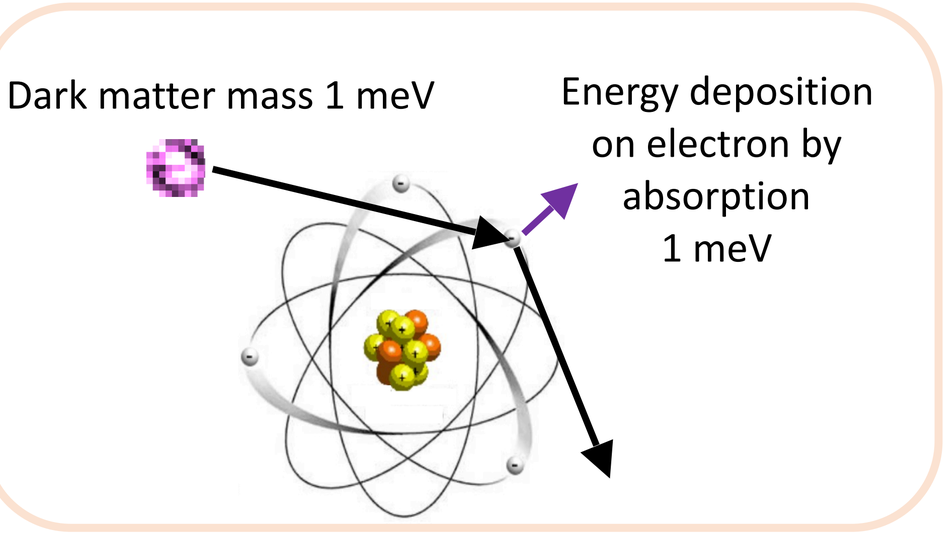
Spin-orbit semiconductors for dark matter detection

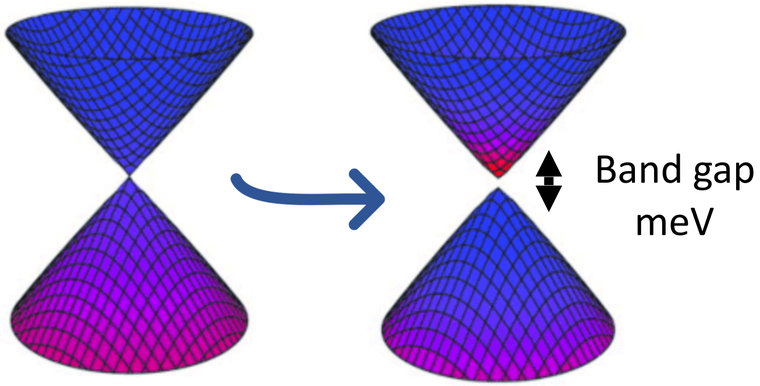
Inzani, **Griffin**



- Direct detection of sub-GeV masses is within the reach of short, small-scale experiments
- Small band gap semiconductors could be used to observe absorption or scattering events

Aim: To identify semiconductors with millielectronvolt band gaps





Effect of spin-orbit coupling

Strategy: Search for materials with band gaps opened by spin-orbit coupling

Spin-orbit semiconductors for dark matter detection

Inzani, **Griffin**

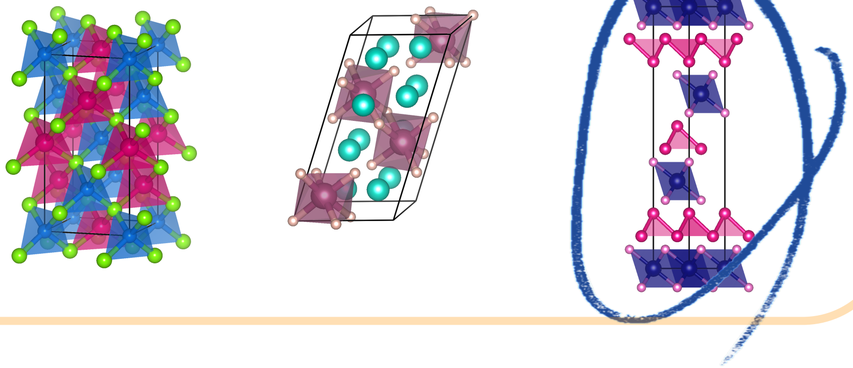
Method I: High-throughput computational screening

MATERIALS PROJECT

86,412 inorganic materials

Spin-orbit interactions in **4,357** compounds

3 "would-be metals" with band gaps opened up through spin orbit coupling



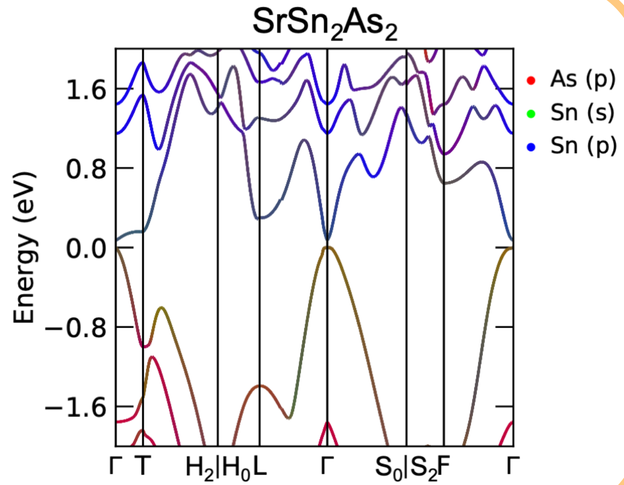
Method II: Refined electronic structures calculated by density functional theory

1 Family of materials with meV-scale band gaps

Tin pnictides $A\mathrm{Sn}_2Pn_2$

Band gap variable by composition

0 – 200 meV



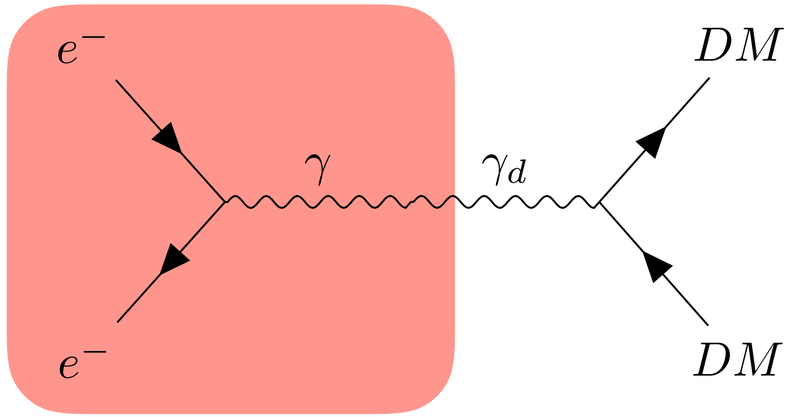
Candidate materials for dark matter detection identified

Synthesis pending…

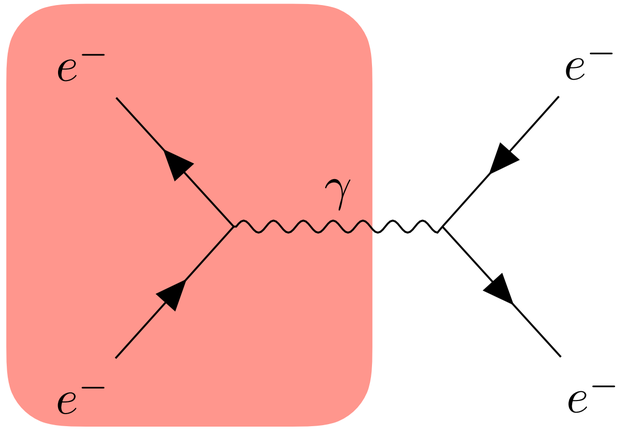
Part 2: determining detection limits

Scattering

Dark matter scattering through a dark photon



Electron energy loss scattering



$$\mathrm{Im}\frac{1}{\epsilon(q,\omega)}$$

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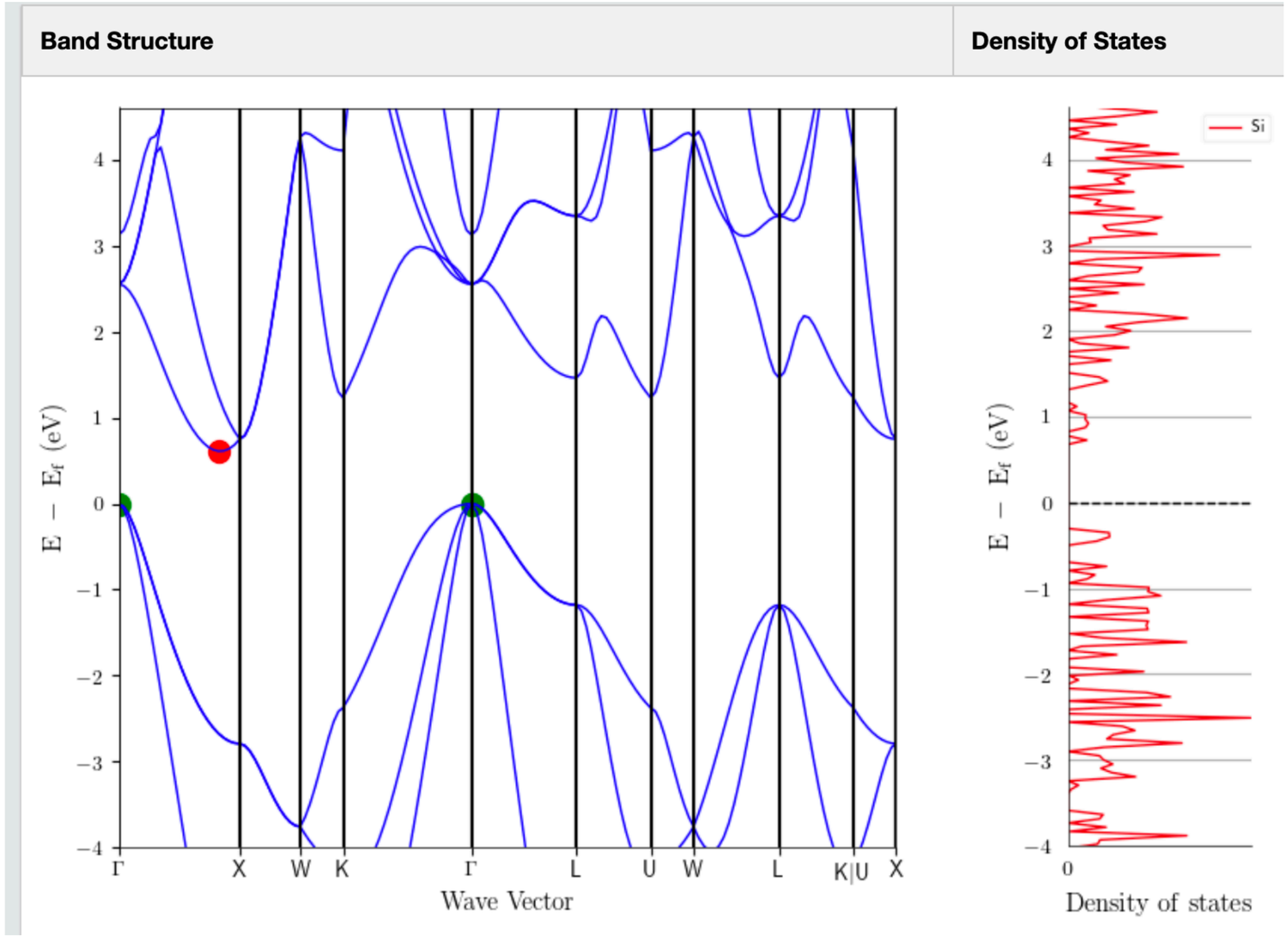
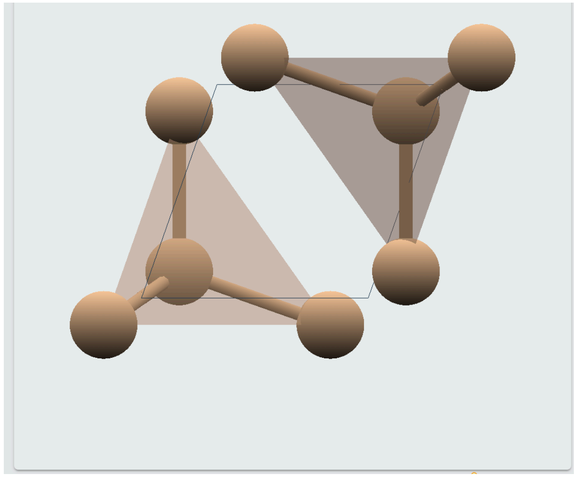
Computation of properties





The band structure is a lie

Materials are collections of many particles and all excitations are many-particle excitations.

pictures from materialsproject.org

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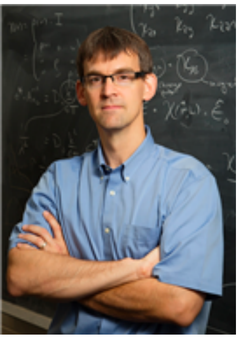


General points about the electron form factor

First approximation to the electron form factor:

$$F_e = \sum_k \left| \int dr^3 \psi^*_{k+q}(\mathbf{r}) \psi_k(\mathbf{r}) e^{-i\mathbf{q}\cdot\mathbf{r}} \right|^2 \delta(\omega - \omega_{k+q} + \omega_k)$$

Bloch states (e.g., from a DFT package)

Energy conservation

General electron form factor is the van Hove function:

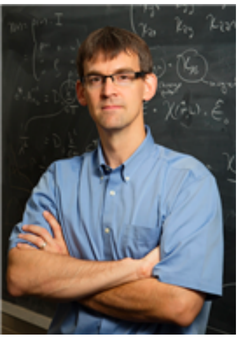
$$S(q,\omega) = \sum_{n,m} \left| < n \mid \hat{\rho}_q \mid m > \right|^2 P_m \delta(\omega - \omega_n + \omega_m)$$

Many-body wave functions

Density operator

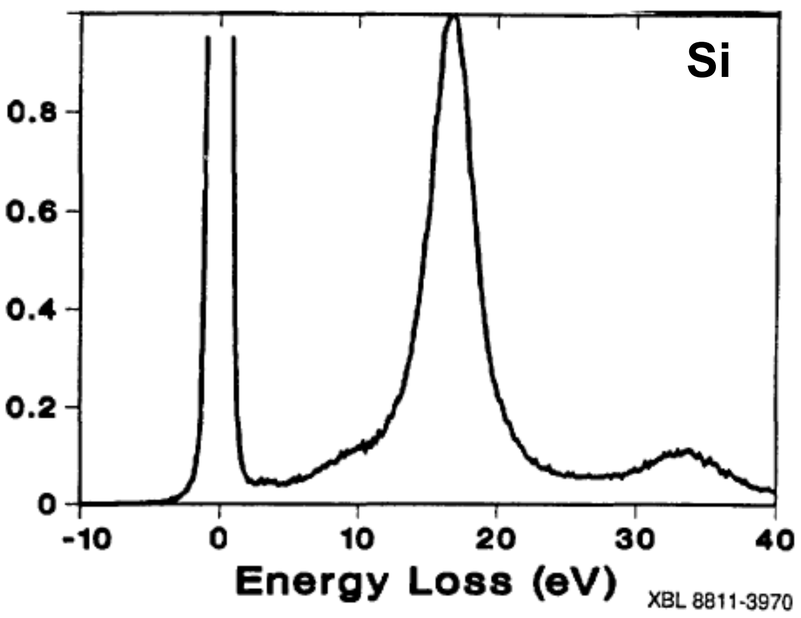
Boltzmann factor if T≠0

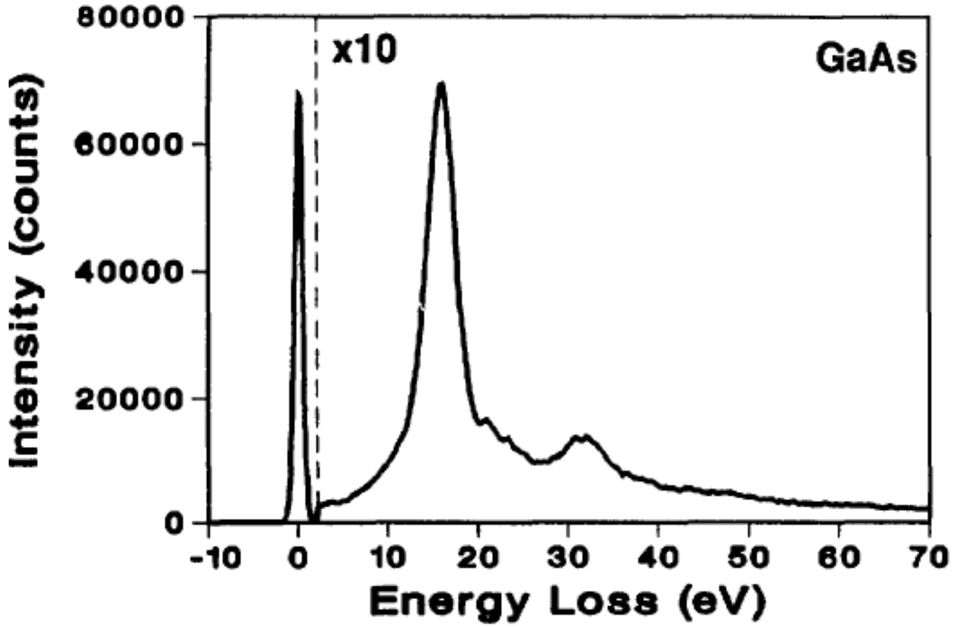
Still need this, of course



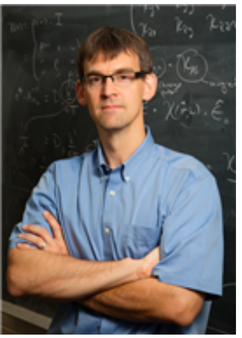
Loss functions for Si vs. GaAs

- Interactions shift spectral weight to the plasma frequency
- $S(q,\omega)$ for Si and GaAs are nearly the same and peaked at 15 eV
- Choosing DM target requires accounting for RPA-like effects

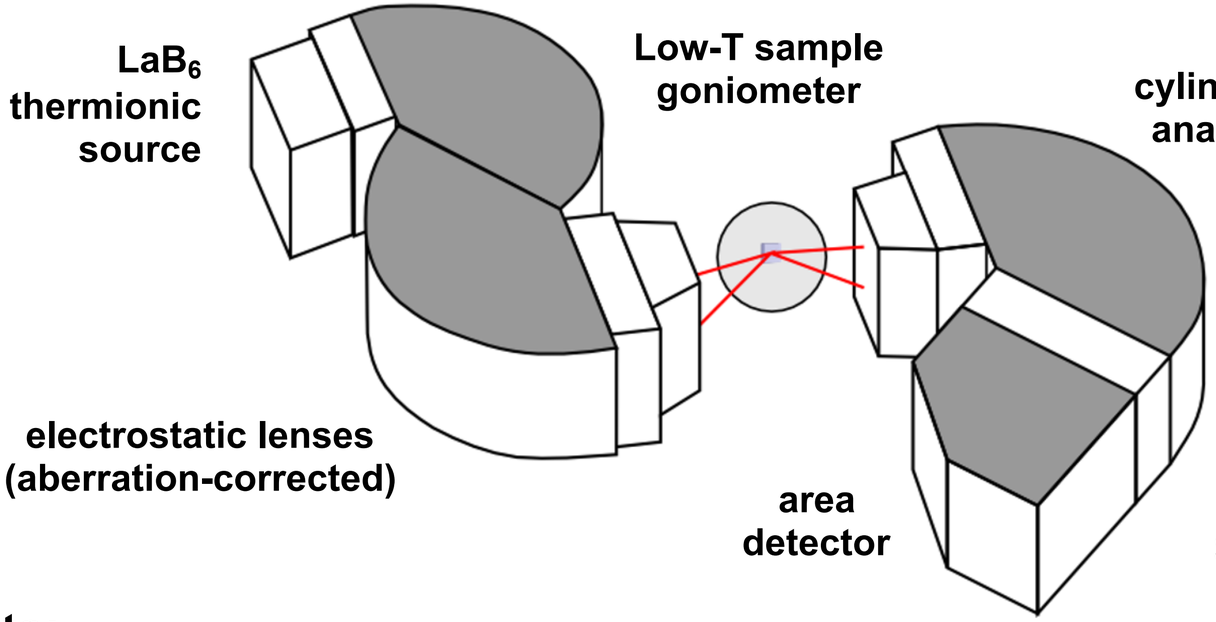




M. K. Kundmann, Ph.D. Thesis, U.C. Berkeley, Nov. 1988



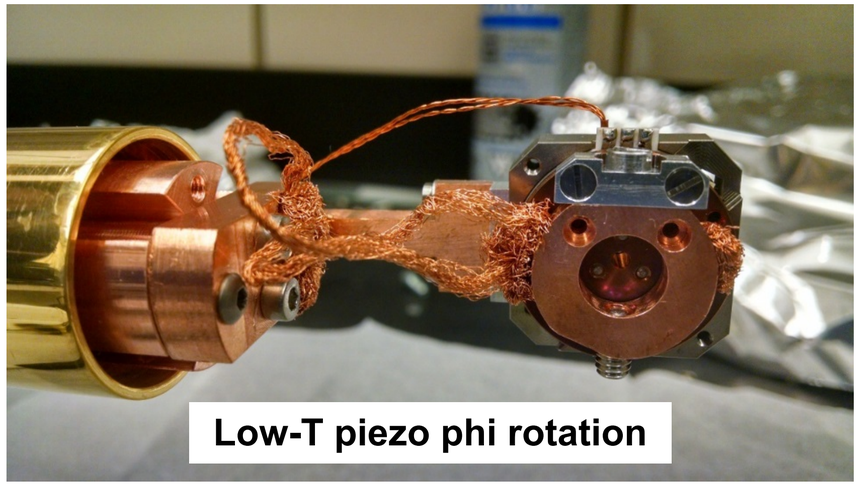
M-EELS facility at UIUC



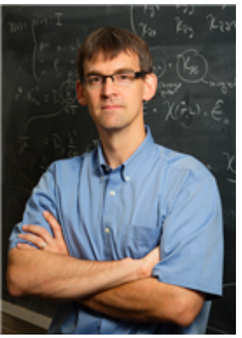
S. Vig, et al., SciPost Phys. **3**, 026 (2017)

Key points:

- **cameras + axes to center the stages**
- **$\Delta q_{acc} \approx 0.013$ Å^{-1}, $\Delta q_{res} \approx 0.02$ Å^{-1}**
- **2.2 meV energy resolution**
- **Measures electronic modes**
- **Surface probe: Works on 2D materials, single layers**



P. Abbamonte, UIUC



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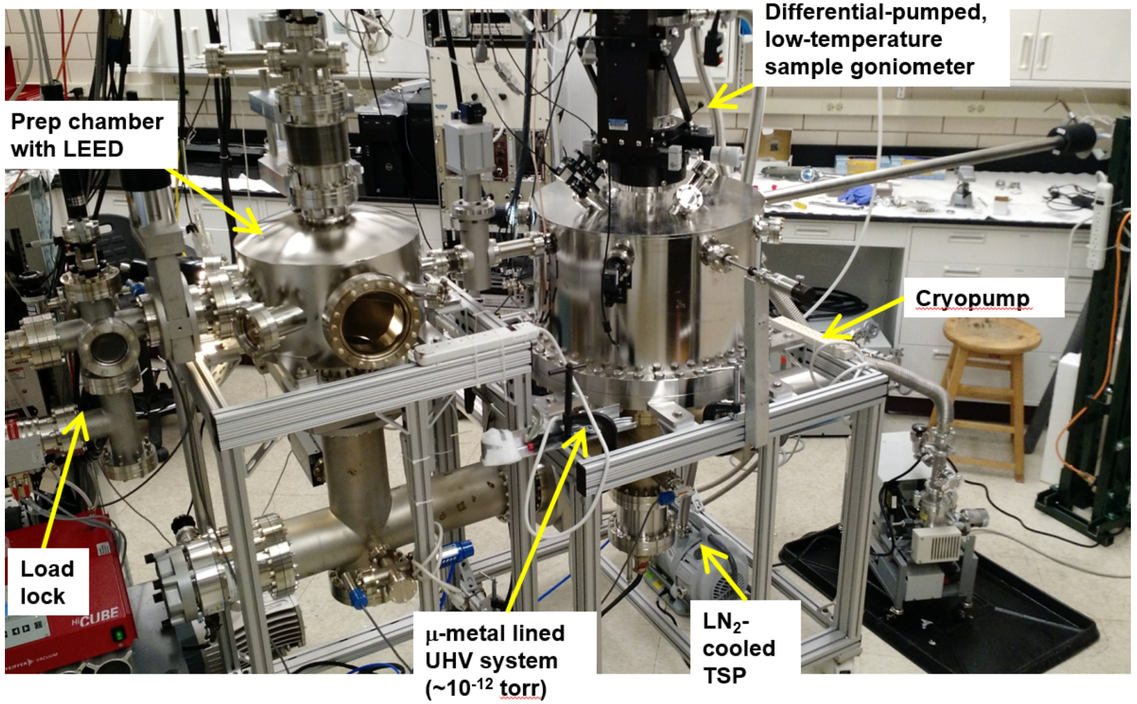

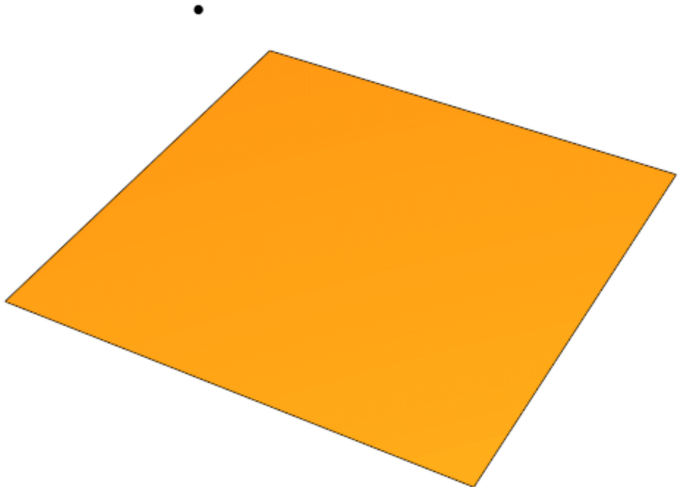

M-EELS measures the *surface* dynamic charge susceptibility:

$$\frac{\partial^2\sigma}{\partial\Omega dE} = \sigma_0 \left[V_{eff}(k_i^z, k_s^z, q)\right]^2 \cdot S(q,\omega)$$

$$S(q,\omega) = -\frac{1}{\pi}\frac{1}{1-e^{-\hbar\omega/k_BT}} \cdot \chi''(q,\omega) \sim -\mathrm{Im}\frac{1}{\varepsilon(q,\omega)}$$

* S. Vig, et al., SciPost Phys. **3**, 026 (2017)

Summary

There are lots of materials. Materials Genome is about sifting through them.

Materials are many-body objects. All excitations are collective.

All effective models are approximate and the ‘cutoff’ can be very small.

Computing properties and response accurately can be challenging but progress can be made with work

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