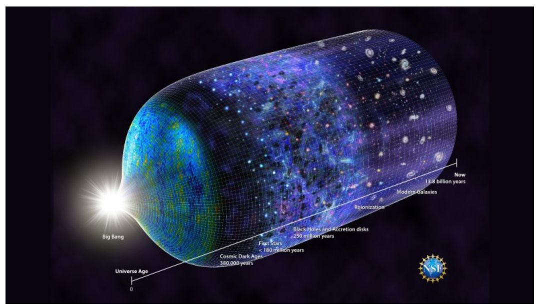
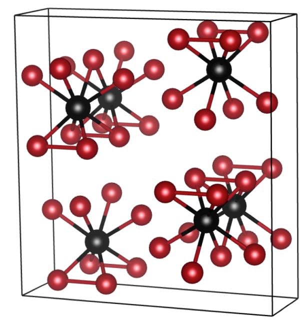
Optical Phonon R&D

Or

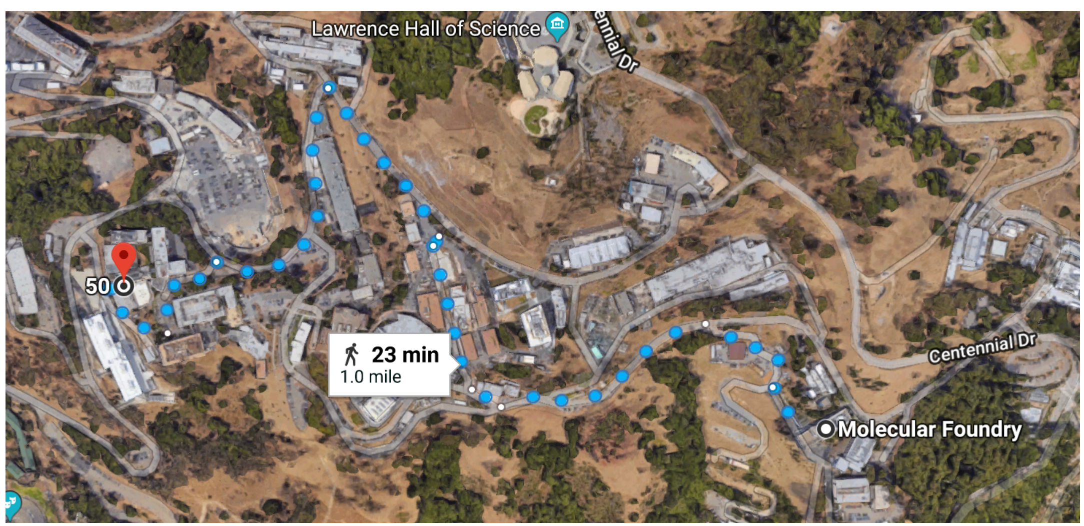
What Condensed Matter Theory/Computation Can do For You

Light years



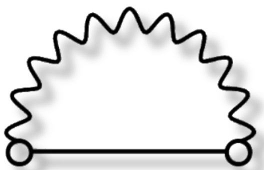


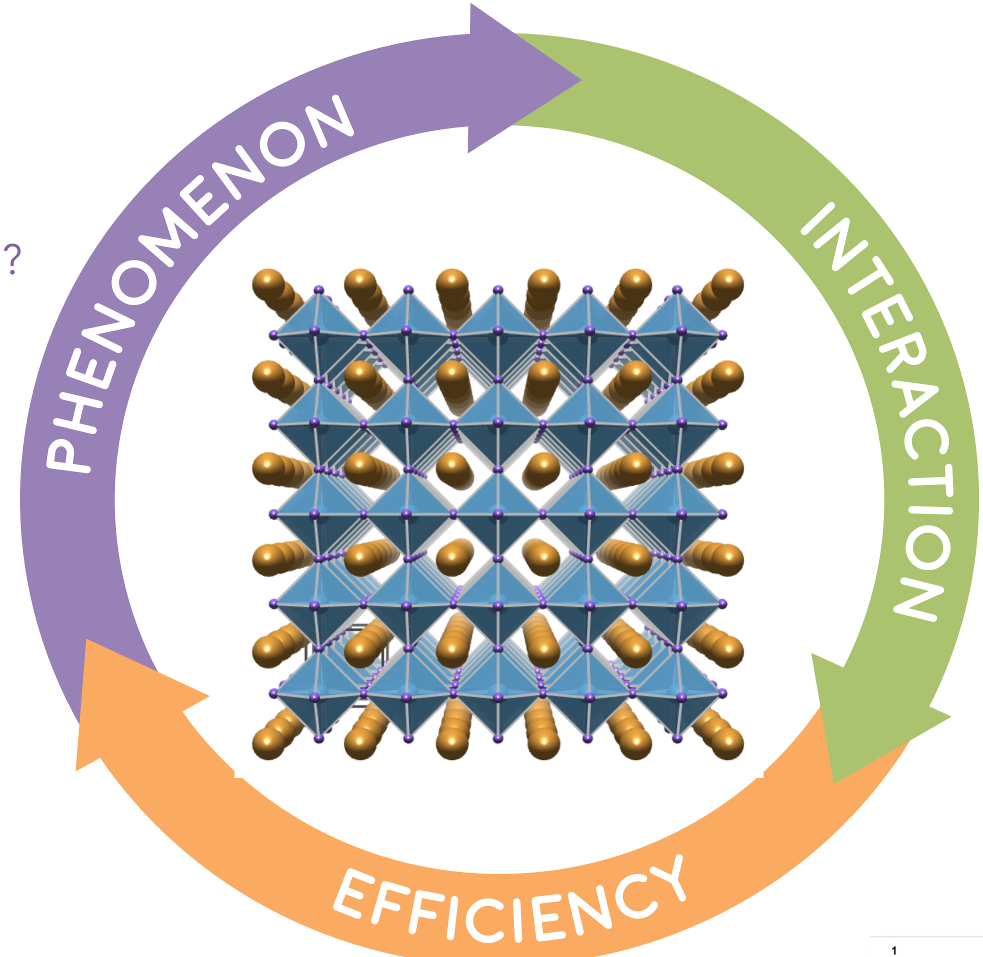
Nanometers



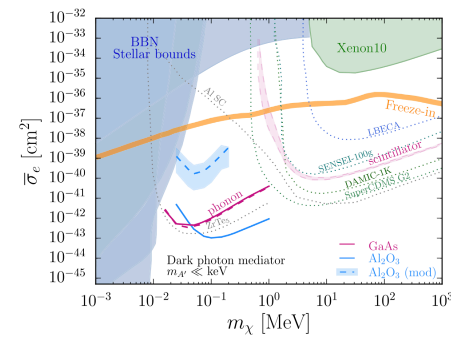
Target Theory and Design

What phenomena?
What materials?



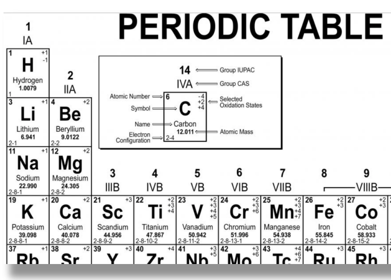


Strength of mechanism
Reach estimates



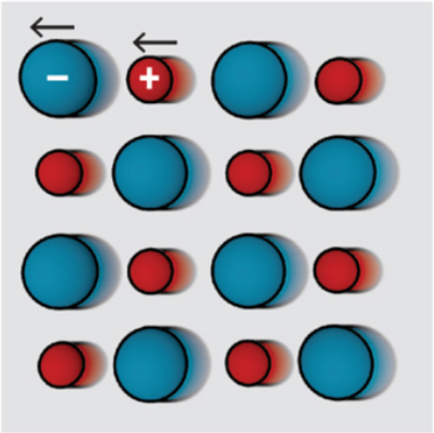
DFT+beyond (Density functional theory)
Symmetry analysis
Effective Hamiltonians

Target efficiency
Optimize interaction/reach

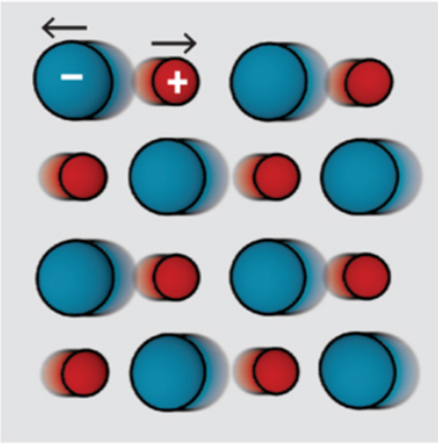


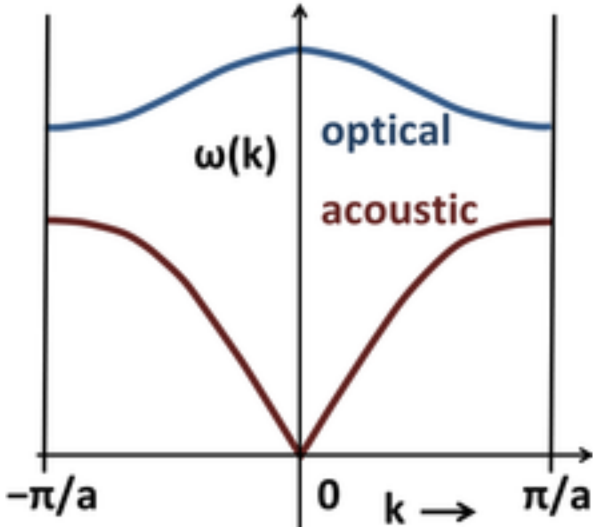
Phonons are Lattice Vibrations

Acoustic Phonons



Optical Phonons

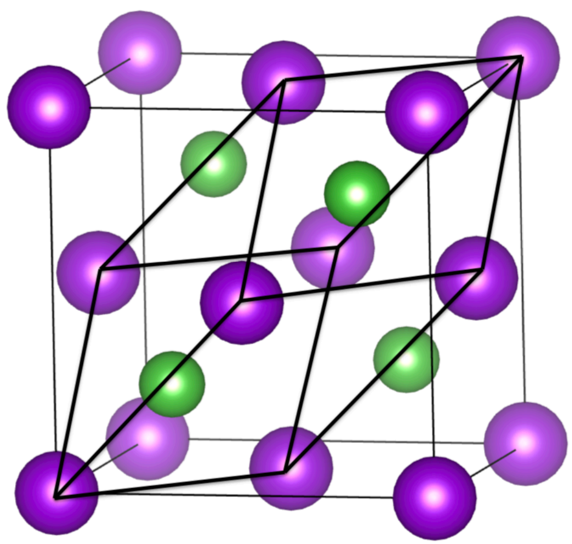




What are Polar Materials?

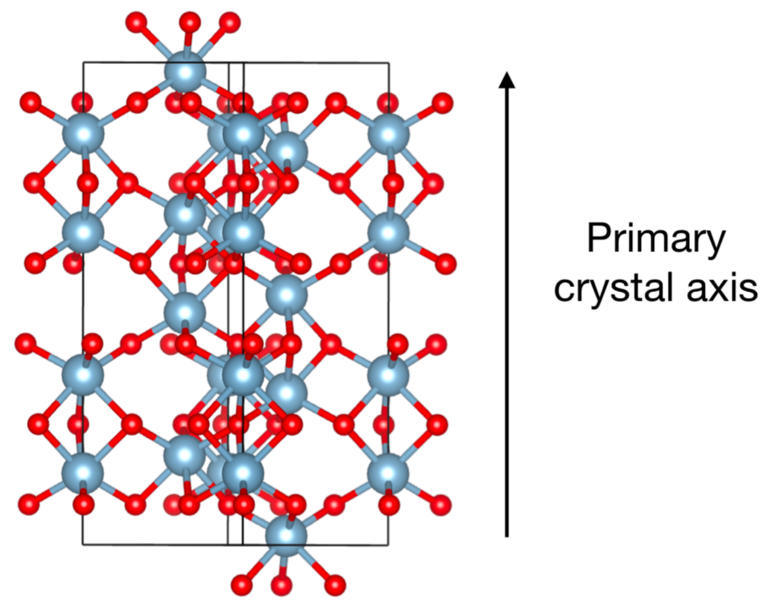
- At least two different ionic species
- Local **dipole** moment

GaAs



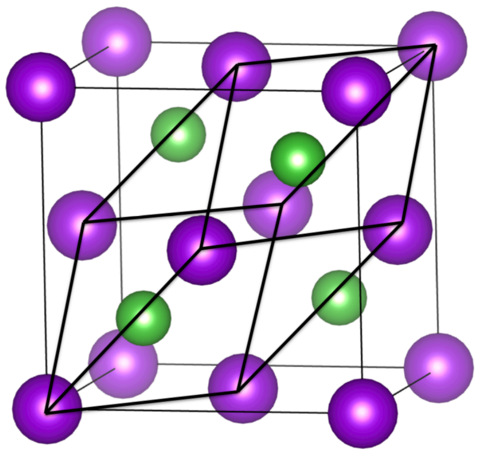
2 atoms in primitive cell

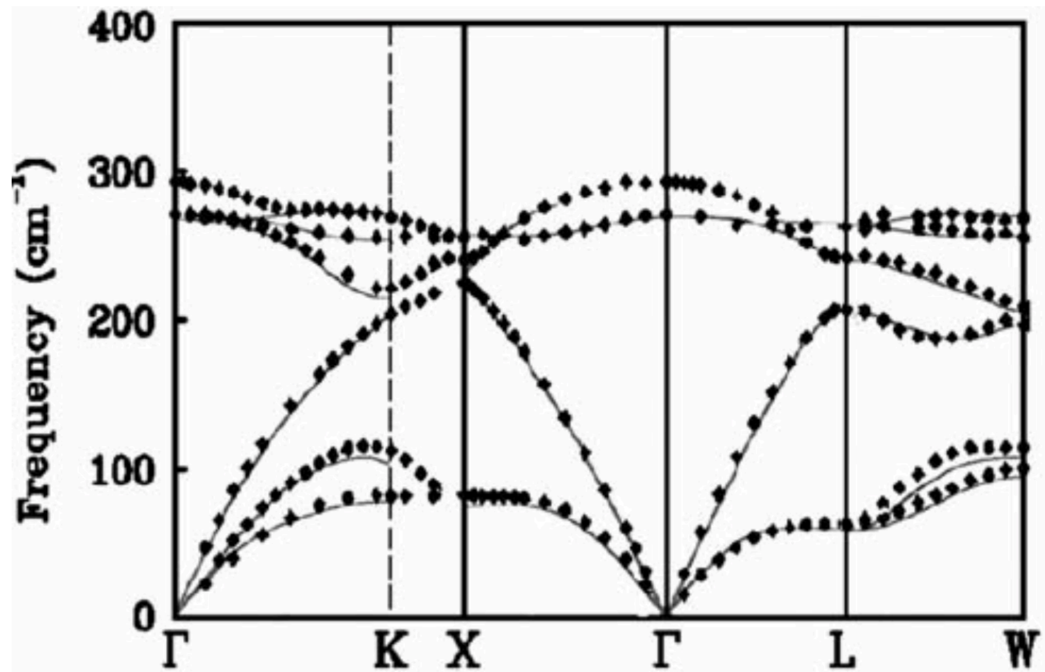
Al_2O_3 (Sapphire)



10 atoms in primitive cell

Why Polar Materials?





From Strauch & Dorner, JPCM 2 1457 (1990)

1. **Kinematic matching** with optical phonons
2. Small screening (insulating or semiconducting)
3. Can have anisotropic crystal structure (directional detection)
4. High-quality crystals available now

Discussing DM absorption via dark phonon with optical phonons

Fröhlich Hamiltonian – DM/phonon interaction

$$H = i\frac{\kappa e^2}{V}\sum_{j,\upsilon,\mathbf{q}}\sum_{\mathbf{G}\neq\mathbf{q}}\frac{1}{\sqrt{2Nm_j\omega_{\nu,q}}}\frac{(\mathbf{q}+\mathbf{G})\cdot\mathbf{Z_j}\cdot\mathbf{e_{j,u}}(\mathbf{q})}{(\mathbf{q}+\mathbf{G})\cdot\varepsilon_{\mathbf{inf}}\cdot(\mathbf{q}+\mathbf{G})}e^{i(\mathbf{q}+\mathbf{G})\cdot(\mathbf{r}+\tau_j)}$$

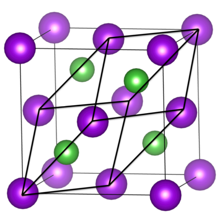
Born effective charge

Phonon eigenvectors

Sum over BZ

Phonon energy

High-frequency dielectric constant

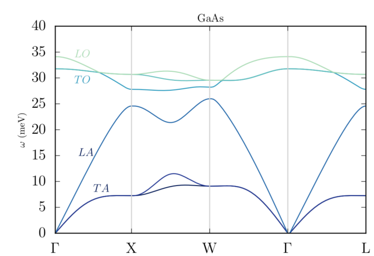


VASP

DFT
E, wavefunction

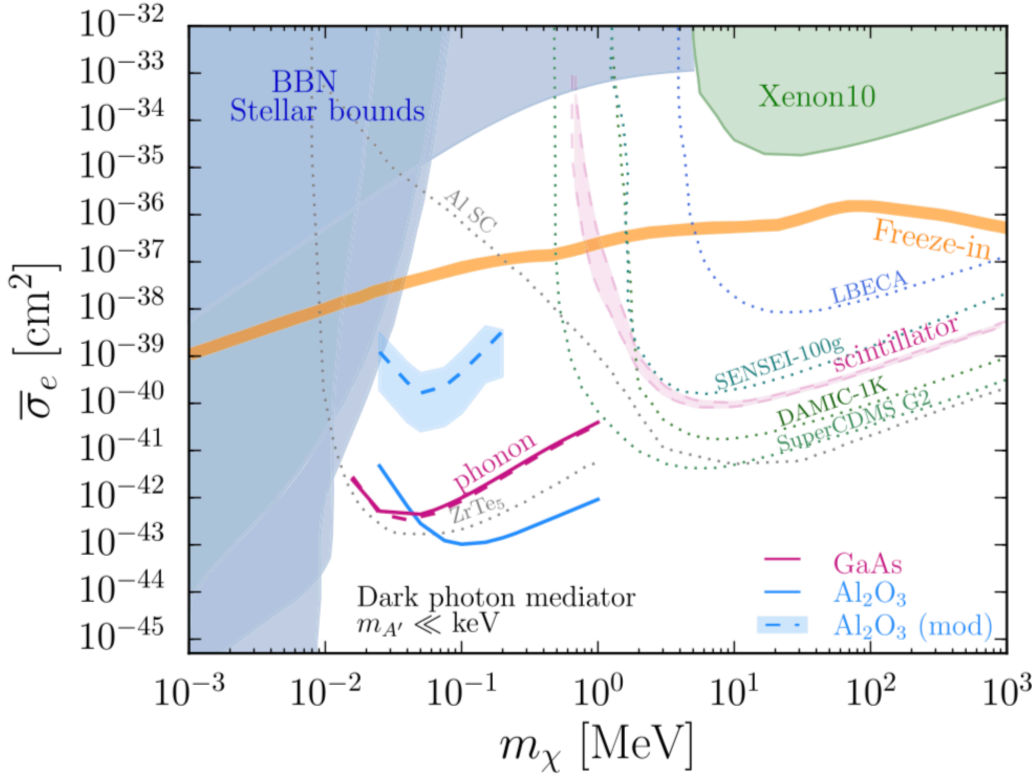
phonopy

Force constant matrix



Theoretical reach of optical phonons

1kg year exposure

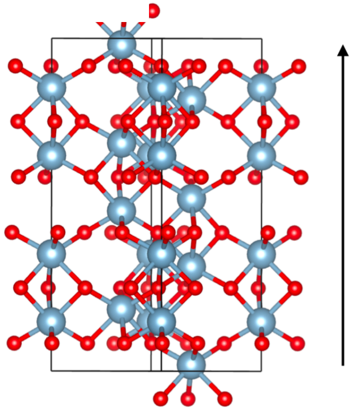



Tongyan Lin, UCSD


Simon Knapen, IAS


Kathryn Zurek, LBL

Hidden bonus: **directionality**!



Can we do better?

$$Q = \frac{Z^{*2}}{A_1 A_2 \varepsilon_\infty^2 \omega_{LO}}$$

Z*= Born effective charges
A_1, A_2= atomic mass numbers
ε_{inf} = high-frequency dielectric constant
w_{LO} = optical phonon frequency

	Z*	A_1	A_2	Eps_inf	w $_{LO}$ (meV)	Q (E-7)
GaAs	2.27	69.7	74.9	10.89 (14.8)	25, 35	2.4
Al_2O_3	2.98, 1.34	27.0	16.0	3.3	30, 106	80

Kevin Zhang, LBL

Tanner Trickle, LBL

Kathryn Zurek, LBL

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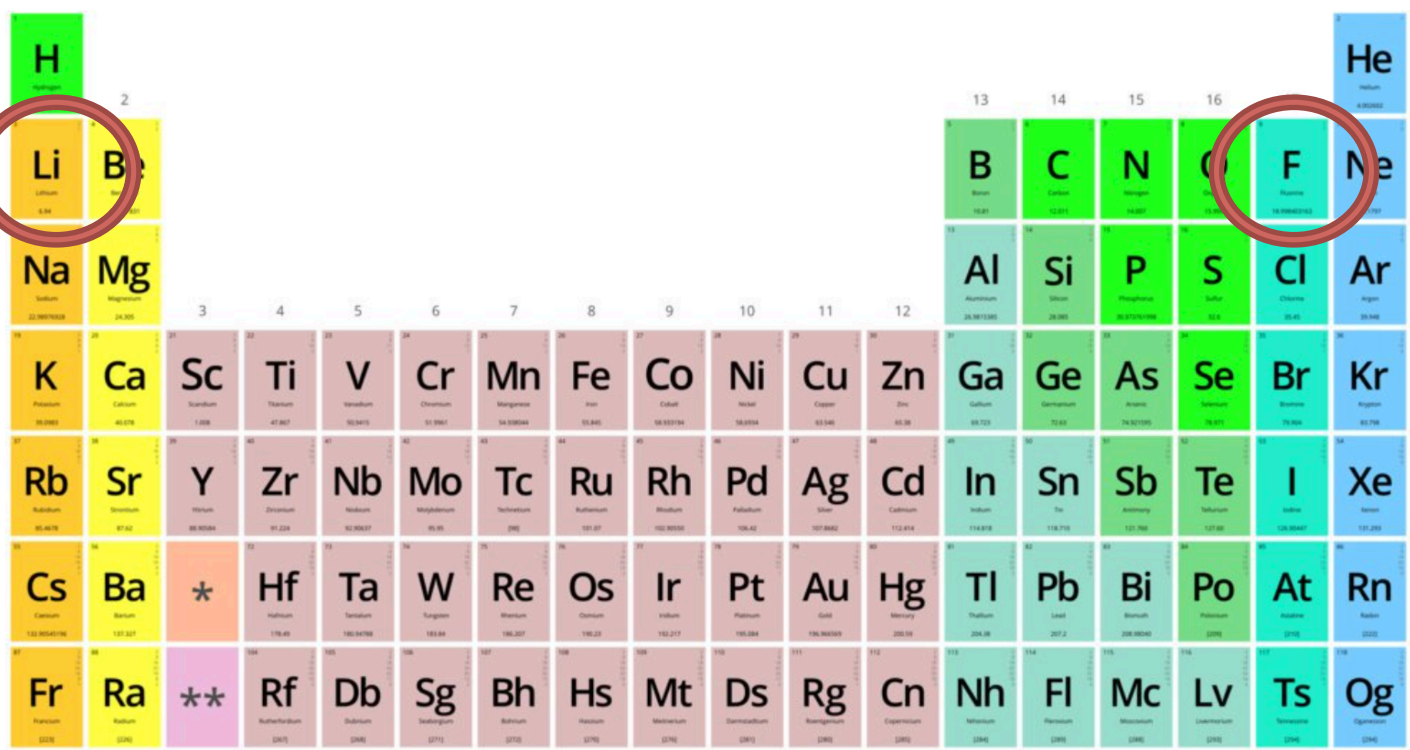
Smaller ions?



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LiF	1.05	6.9	19.0	2.02	77	268

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Materials with large electric polarization?

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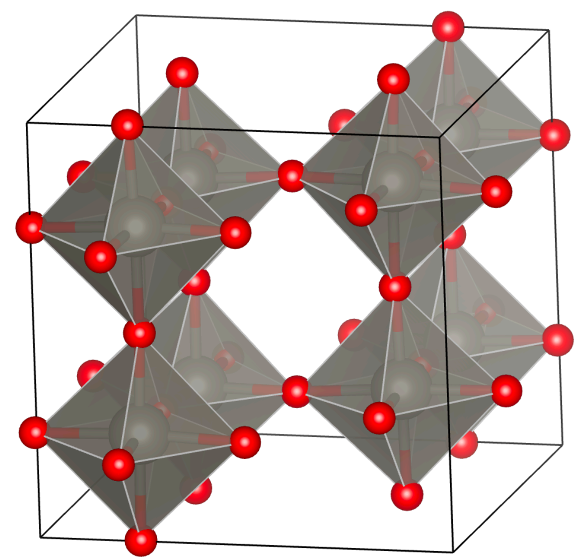
Materials with large electric polarization?

WO_3 (in P4mm structure)
Calculated polarization of **69 μC.cm^{-2}** (high)

Hamdi et al. PRB 94, 245124 (2016)



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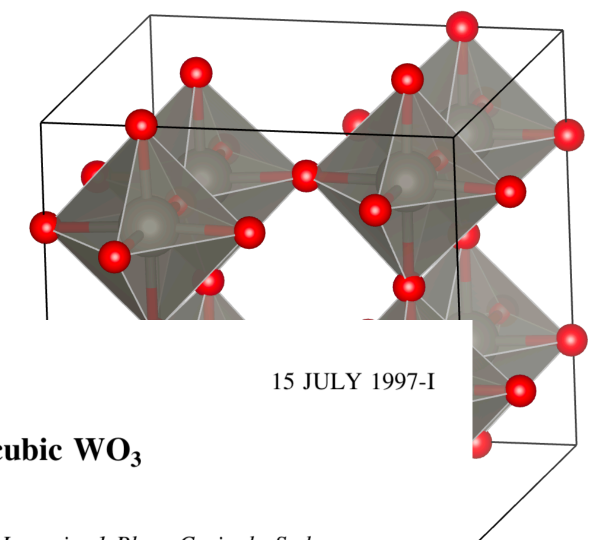

PHYSICAL REVIEW B VOLUME 56, NUMBER 3 15 JULY 1997-I

Anomalously large Born effective charges in cubic WO_3

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(Received 15 January 1997)

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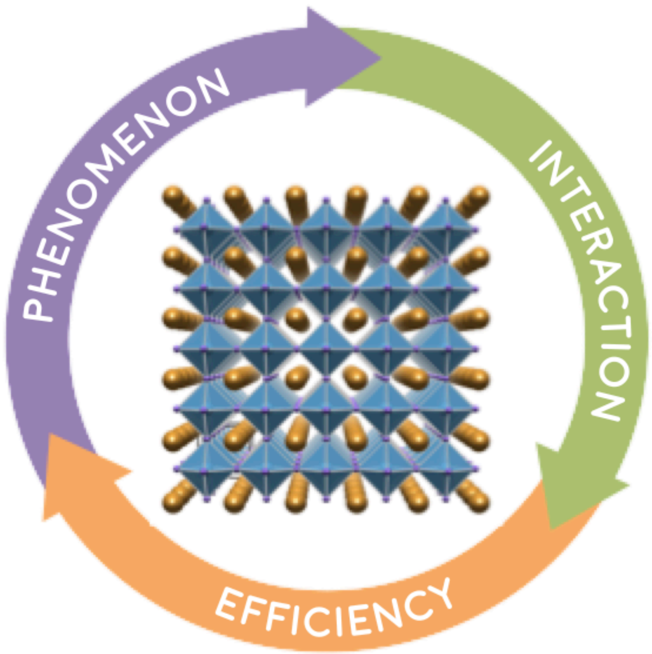
WO_3	11.73, 8.78, 1.62	183.8	16.0	5	126	556

Optical Phonon Theory and Design – Future

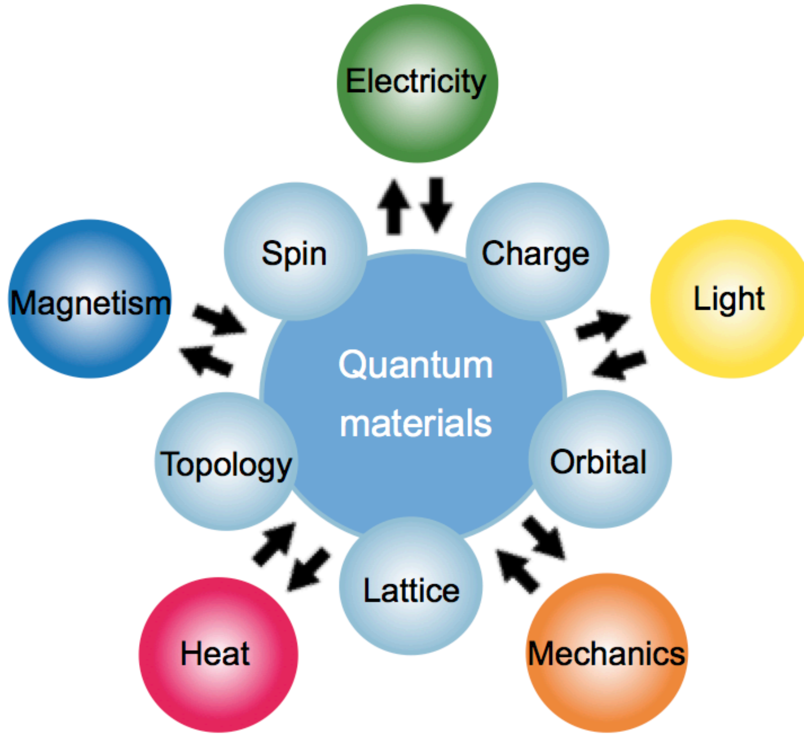


Multi-phonon production
Lin, Knapen
Harrelson, Trickle, Zhang, Zurek

Phonon lifetimes
Harrelson

Better polar semiconductors
Theory and experiment

Ferroelectrics
Lin, Knapen



MOLECULAR FOUNDRY

Characterization		Fabrication	Theory	Synthesis		
NCEM National Center for Electron Microscopy	**Floor 1** Imaging and Manipulation of Nano-structures	**Floor 2** Nano-fabrication	**Floor 3** Theory of Nano-structured Materials	**Floor 4** Inorganic Nano-structures	**Floor 5** Biological Nano-structures	**Floor 6** Organic and Macro-molecular Synthesis
Electron microscopy and nano-characterization	Characterization and manipulation of nanostructures	Advanced lithographic and thin-film processing techniques	Guiding understanding of new principles, behavior and experiments	Science of semiconductor, carbon and hybrid nanostructures	Bio-materials; new probes for bio-imaging; synthetic biology techniques	Soft materials: organics, macromolecules, polymers and their assemblies