Modeling Coating Thermal Noise at Gravitational Wave Detectors

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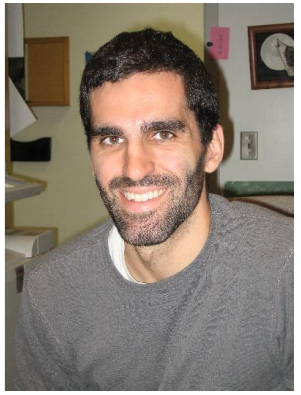
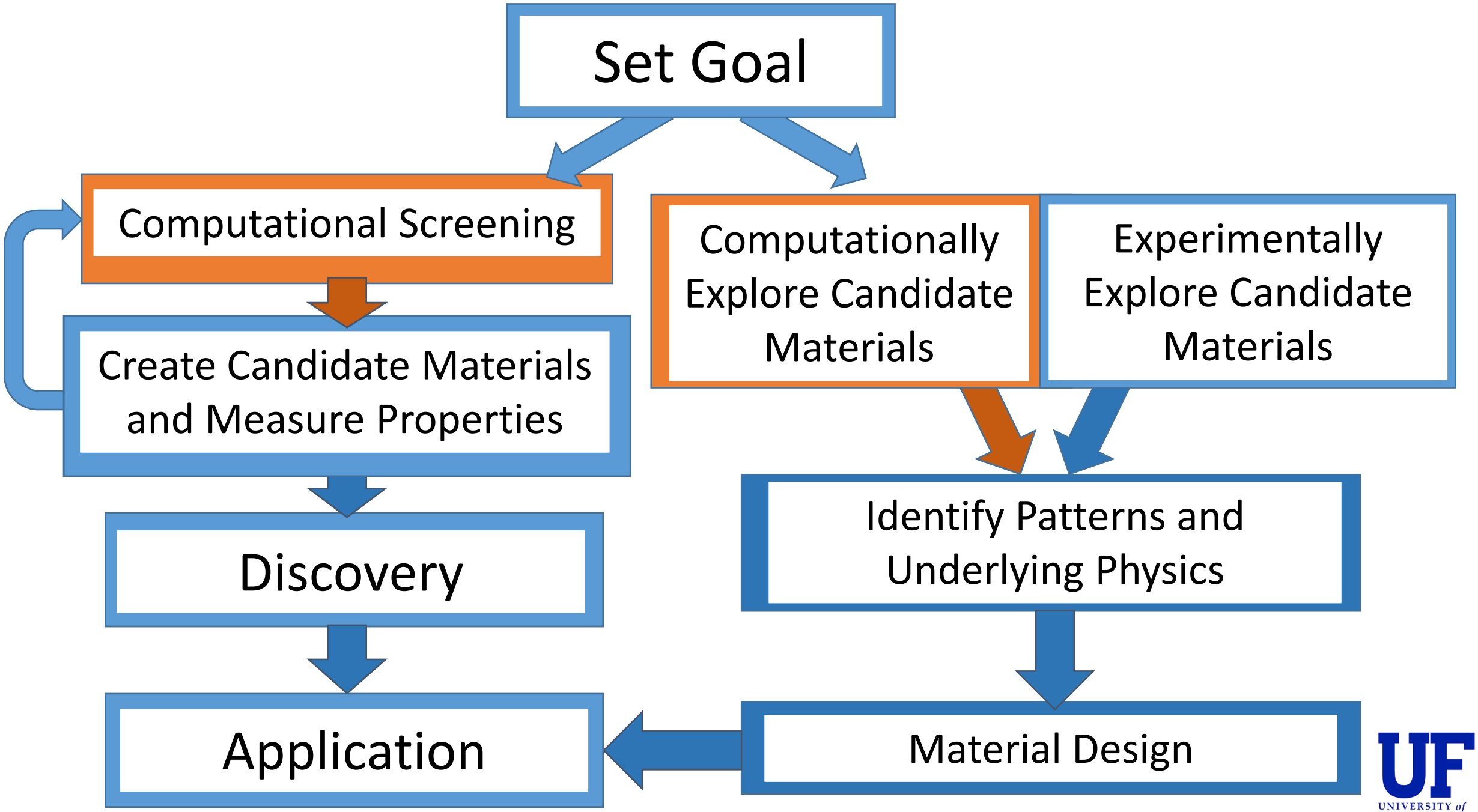
GWADW 5/24/2015





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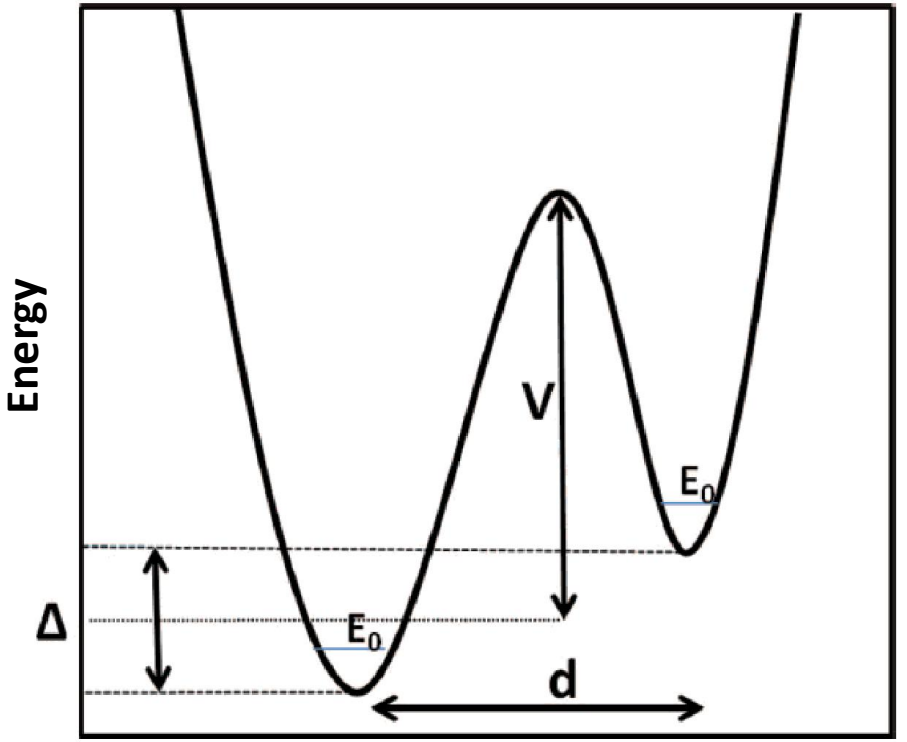
Outline

- Introduction
- Methods
- Results
  - Tantala and Titania-doped Tantala
  - Amorphous Silica
- Current Work
- Conclusion

Two-Level System Model

- The Hamiltonian of the TLS system is:
  $$H = H_1 + (V - V_1) = H_2 + (V - V_2),$$
  - H_i is the Hamiltonian of isolated well *i*
  - V_i is the potential of well *I*



Rashid Hamdan, *J. Phys. Chem* 2014.

- In a localized representation,

$$H = \begin{vmatrix} E_1 + < \varphi_1 | V - V_1 | \varphi_1 > & < \varphi_1 | H | \varphi_2 > \\ < \varphi_2 | H | \varphi_1 > & E_2 + < \varphi_2 | V - V_2 | \varphi_2 > \end{vmatrix}$$

  - where φ_i is the harmonic oscillator wave function
  - E_i is the harmonic oscillator energy in well *i*

Two-Level System: Internal Friction

- Using the relaxation time approximation, we can calculate the internal friction from the imaginary part of the susceptibility to be

$$Q^{-1} = \frac{1}{(3kT)Y} \iint d\Delta dV \frac{\omega\tau}{1+\omega^2\tau^2} \gamma^2 \left(\frac{\Delta}{E}\right)^2 sech^2\left(\frac{E}{2kT}\right) N(\Delta, V)$$

where

- ω is the angular frequency of the wave
- kT is the temperature in eV
- $N(\Delta, V)$ is a number density of TLS's
- γ is the mechanical dipole
- τ is the relaxation time
- Y is the Young's modulus for the system

Usually separated into $N_{TLS} f(\Delta) g(V)$[1]

Usually assumed constant over all TLS's[1]

Calculated using average attempt frequency of all TLS's[1]

1. K. Gilroy and W. Phillips, Philosophical Magazine B 43,735 (1981)

Two-Level System: Internal Friction

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Inputs

- $N(\Delta, V)$ is a number density of TLS's
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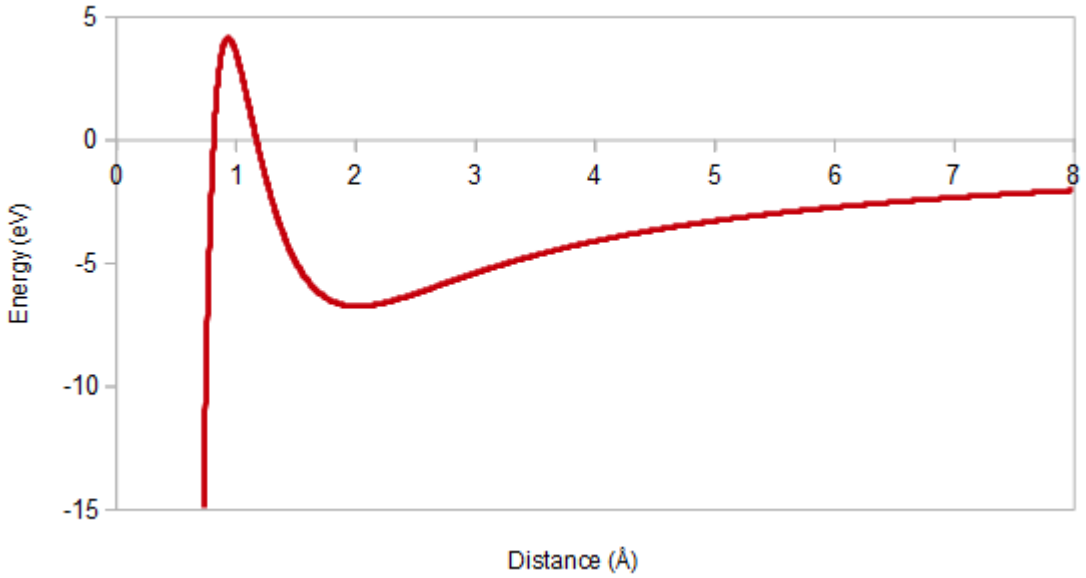
- τ is the relaxation time
- Y is the Young's modulus for the system

Calculated from classical MD

Classical Molecular Dynamics

- Uses Newtonian dynamics to update atomic positions
- Interatomic potentials are modeled to fit experimental data
  - Density
  - Elastic moduli
  - Radial distribution functions
  - Formation energy
- Allows simulations of millions of atoms at low computational cost

$$V_{1-2}(r) = Ae^{-Br} - \frac{C}{r^6} + \frac{kq_1q_2}{r^2}$$



https://en.wikipedia.org/wiki/Buckingham_potential

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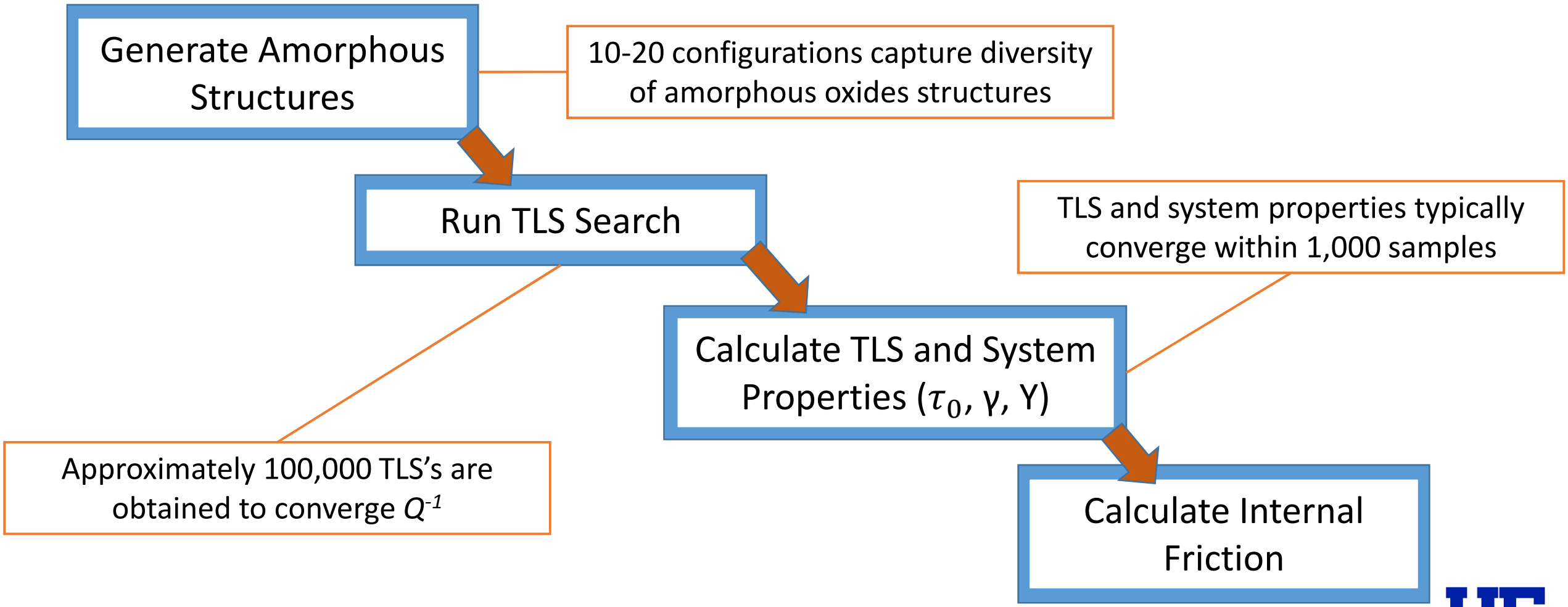
Method Overview



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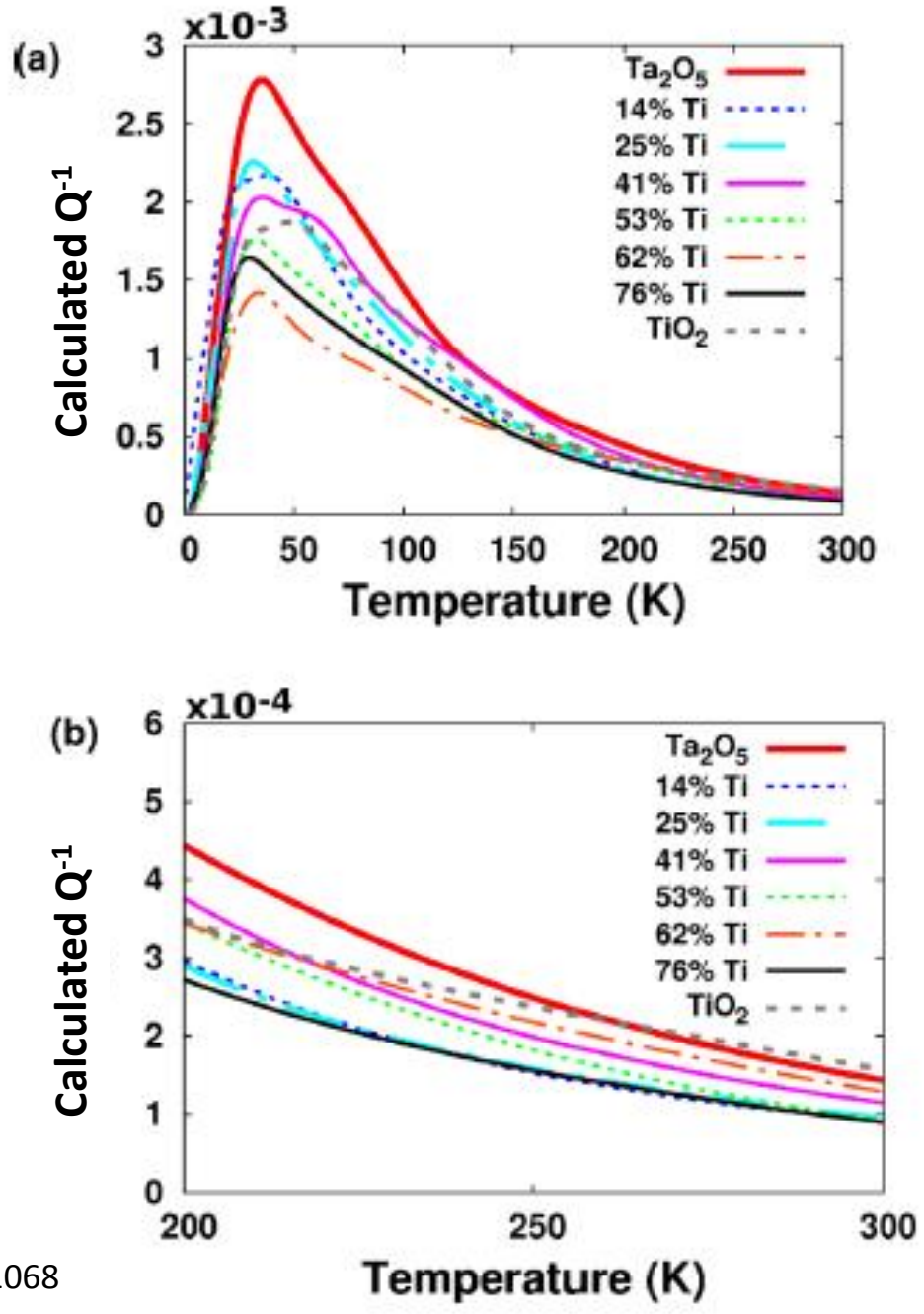
Internal Friction

- Calculated Q^{-1} overestimates measured Q^{-1} by a factor of 2.5, but the trends and shape of $Q^{-1}(T)$ follow experiment
- Percent changes of peak $Q^{-1}(T)$ match experiment quite closely
- For low-T Q^{-1}, optimal value of titania-doping is 62%
- Room-temperature Q^{-1} shows non-monotonic behavior with Ti-doping, but agree with decrease seen in 14% doped experiment



2. JP Trinastic, R Hamdan, C Billman, HP Cheng. *PRB* **93**, 014105 (2016).

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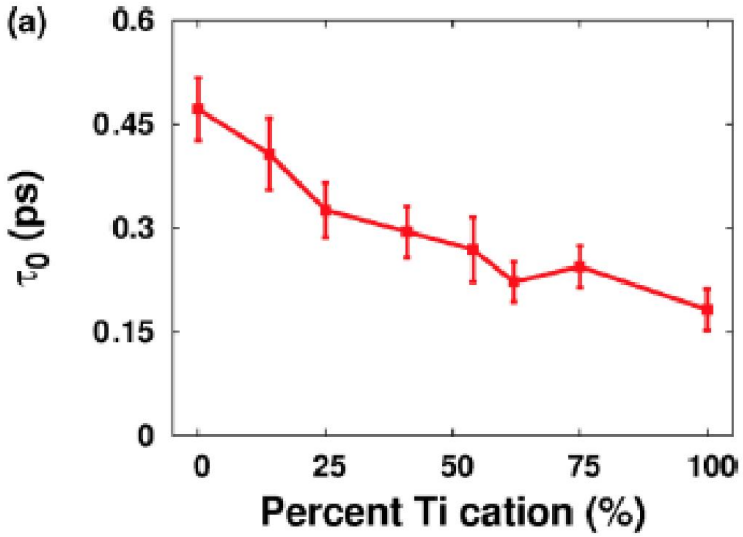
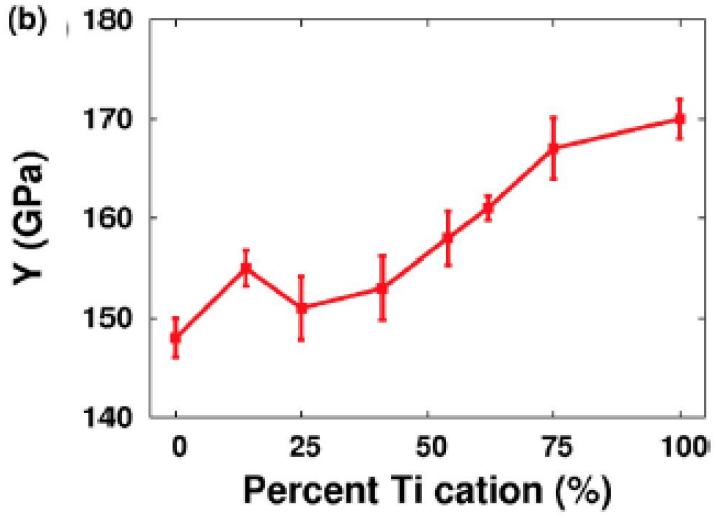
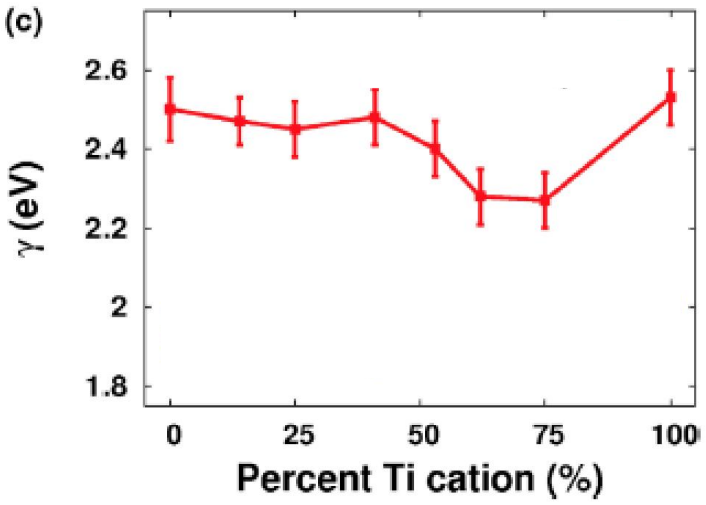
Calculated Q^{-1} Parameters



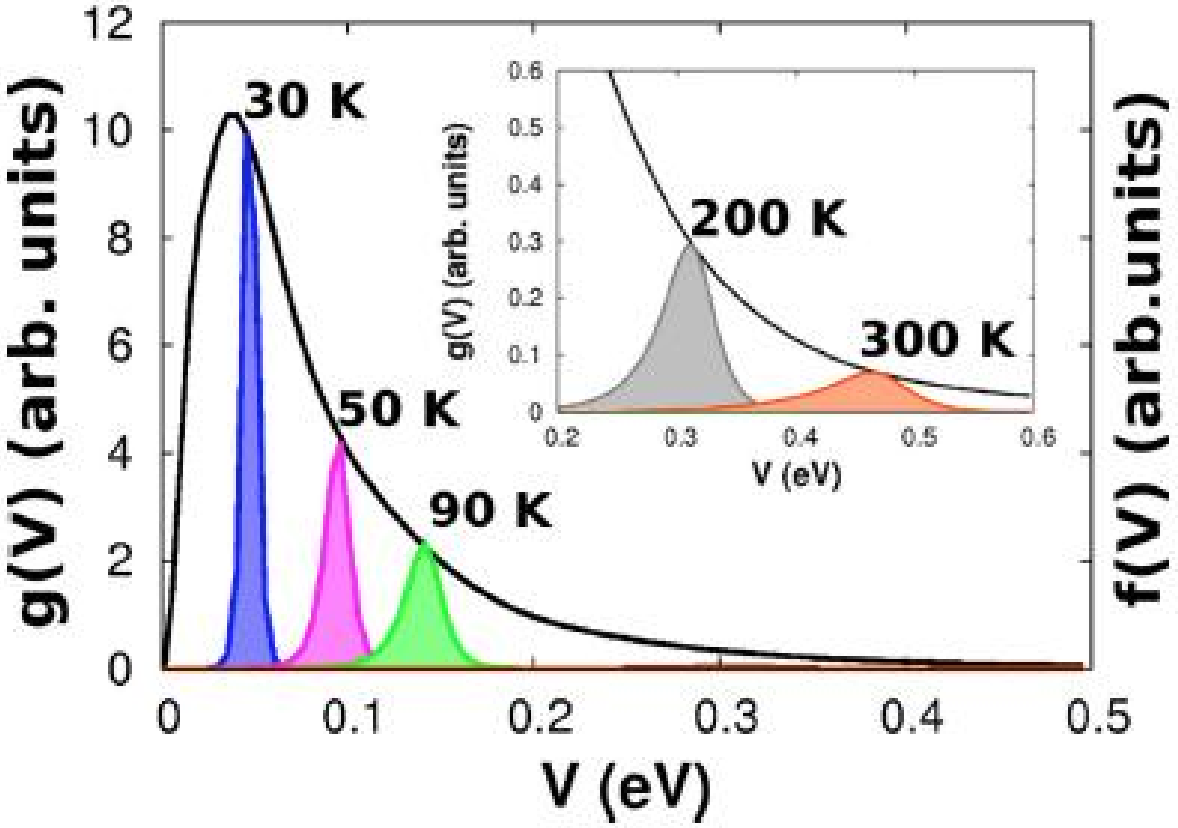




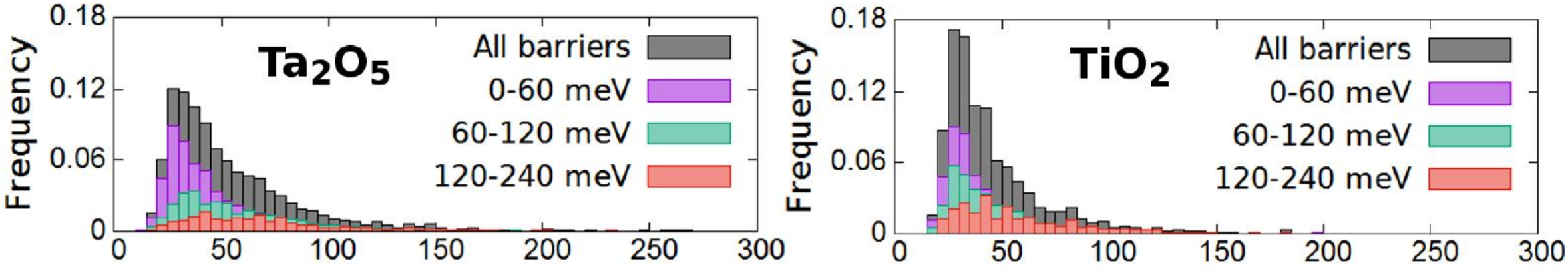
- Ti doping generally corresponds with
  - shorter relaxation time (τ_0)
  - larger Young's modulus (*Y)*
  - weaker longitudinal coupling constant (γ)
- The minimum in γ leads to the optimal doping at 64%
- Controlling the coupling constant through doping is a way to decrease Q^{-1}

TLS Activation

- Regions of $Q^{-1}(T)$ can be connected to TLS's by plotting the expression for Q^{-1} without integrating over V and Δ
- This identifies transitions that lead to loss at a particular temperatures



Statistics of TLS transitions



- Sharper peaks in the number of atoms involved in TiO_2 compared to Ta_2O_5 suggest a more localized transition
- Similar statistics → similar loss mechanism

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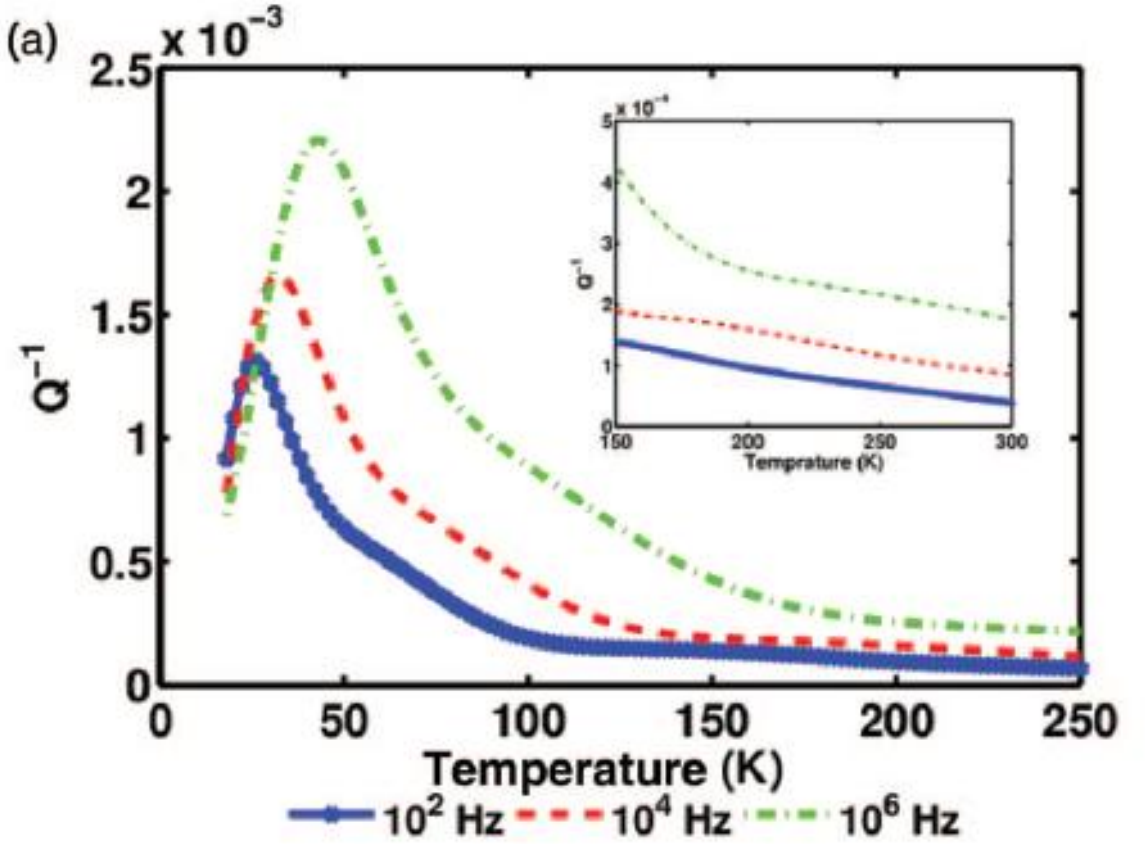
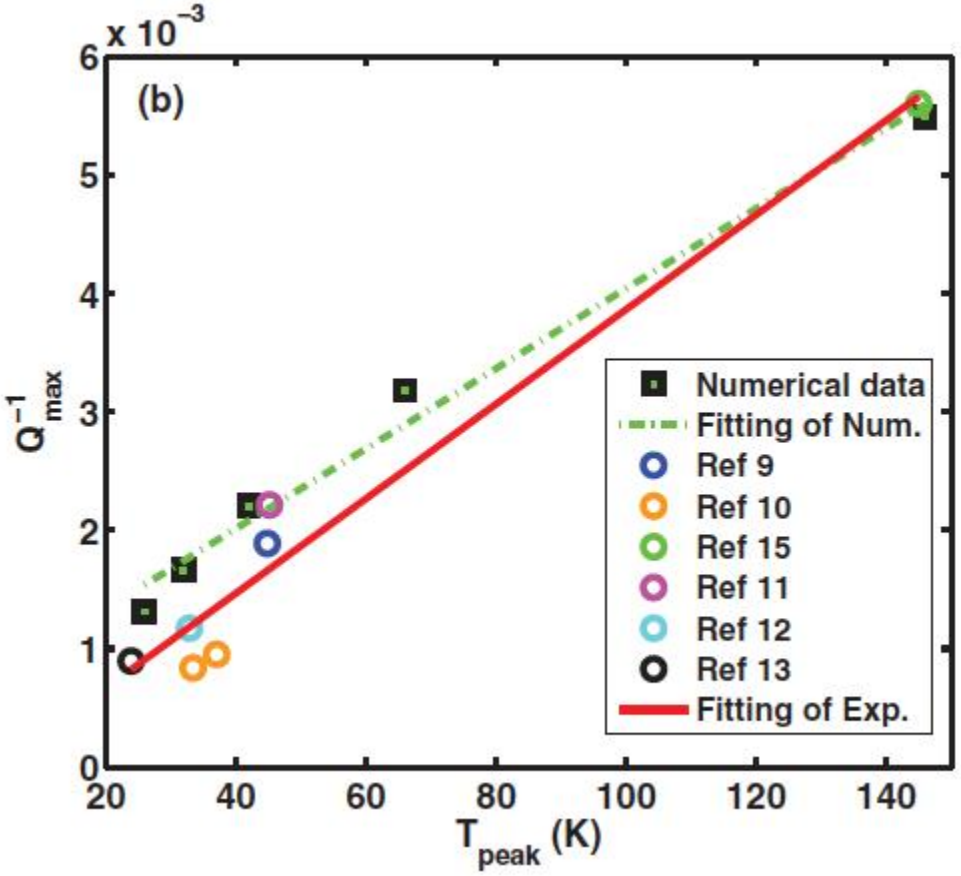
Re-examining Amorphous Silica





Previous calculations gave good agreement for low temperature peak

3. R. Hamdan, J. P. Trinastic, and H. Cheng, The Journal of chemical physics 141, 054501 (2014).

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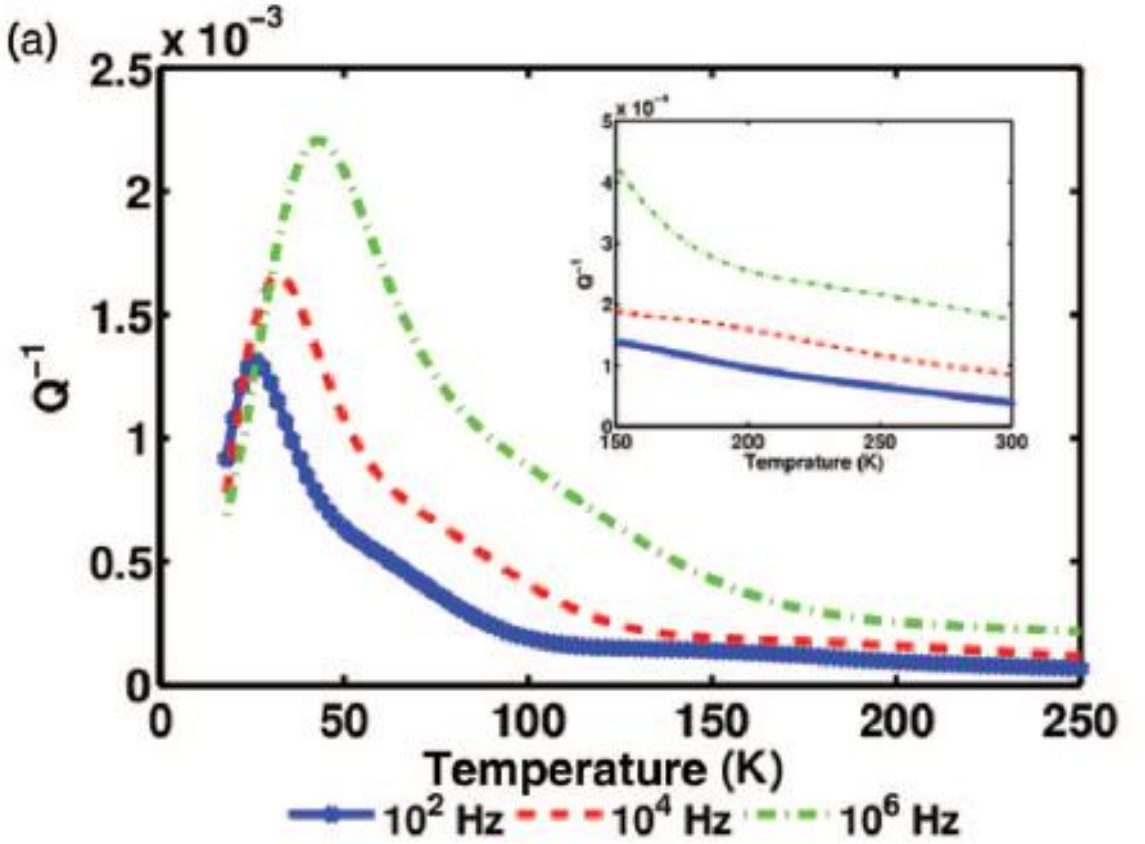
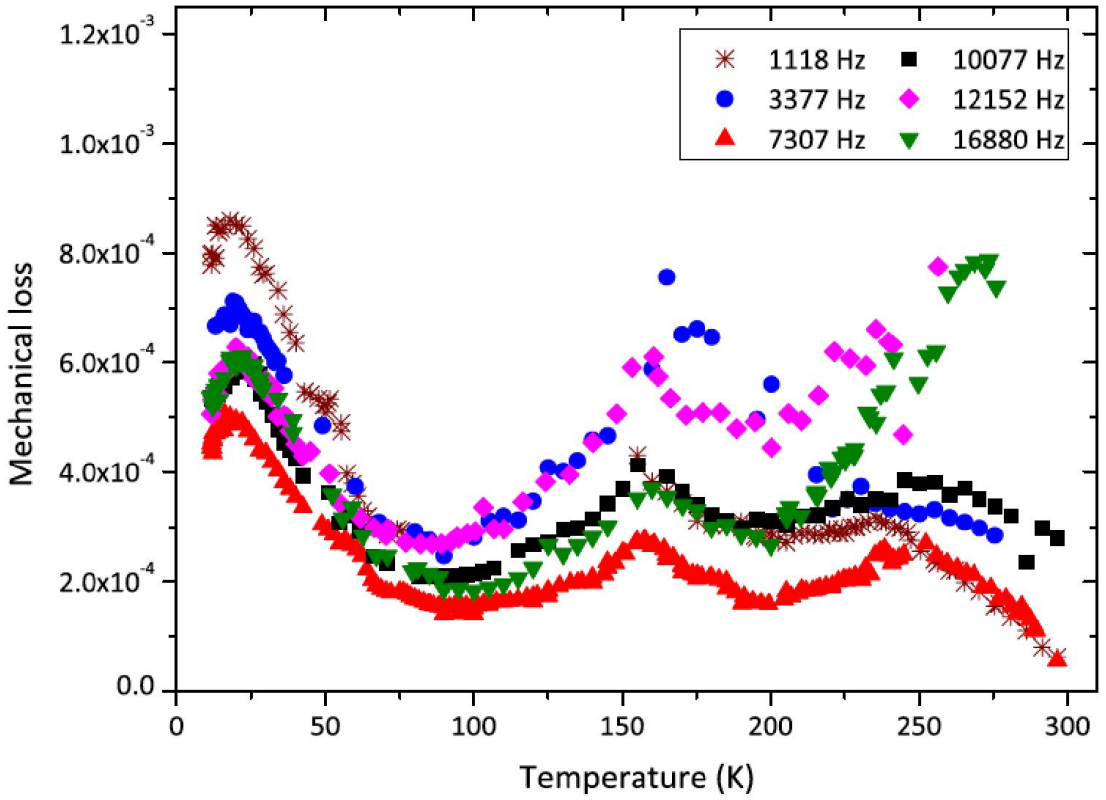
Re-examining Amorphous Silica





Not describing high-temperature behavior well! Why?

3. R. Hamdan, J. P. Trinastic, and H. Cheng, The Journal of chemical physics 141, 054501 (2014).

4. I. Martin, R. Nawrodt, K. Craig, C. Schwarz, R. Bassiri,G. Harry, J. Hough, S. Penn, S. Reid, R. Robie, et al.,Classical and Quantum Gravity 31, 035019 (2014).

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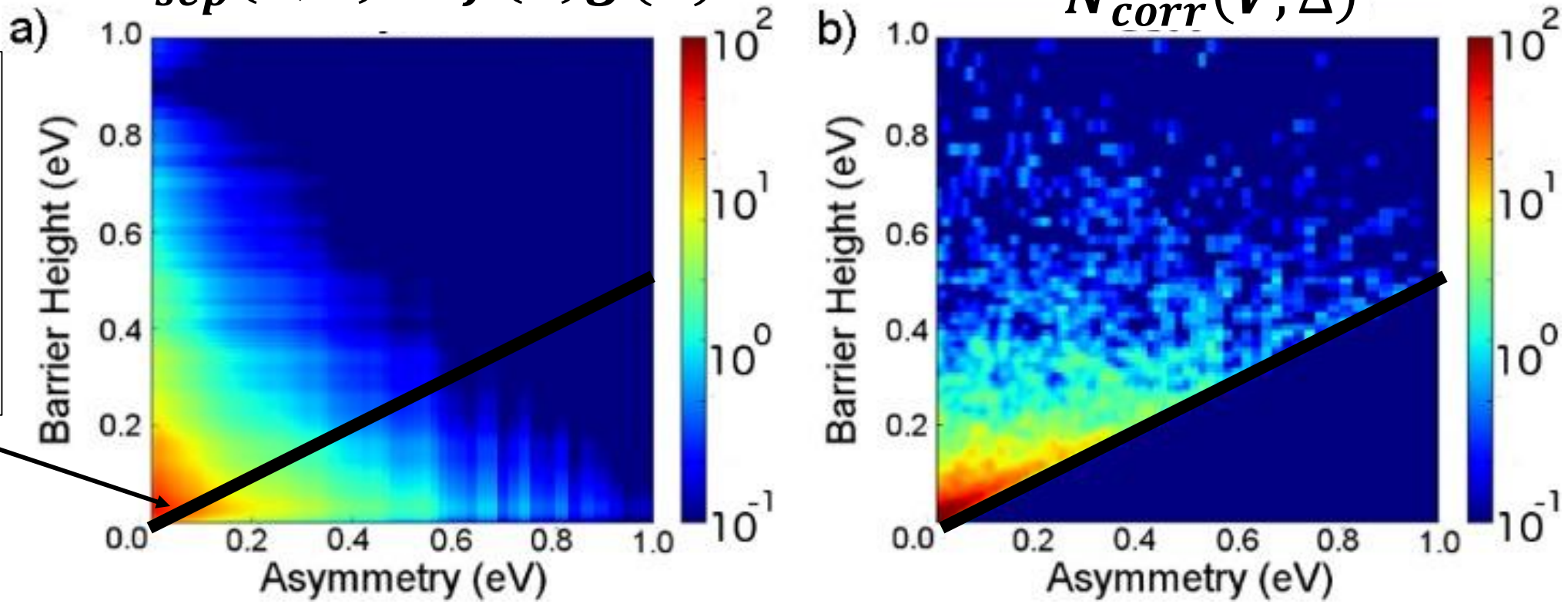
TLS Distributions

$$N_{sep}(V, \Delta) = f(\Delta)g(V)$$

Black diagonal line corresponds to a TLS with zero barrier. A TLS is only defined for the region above the line



$N_{corr}(V, \Delta)$

- Separated distribution gives opposite behavior of the correlated distribution
- Separated distribution has high density below $V < 2\Delta$, violating the definition of a TLS

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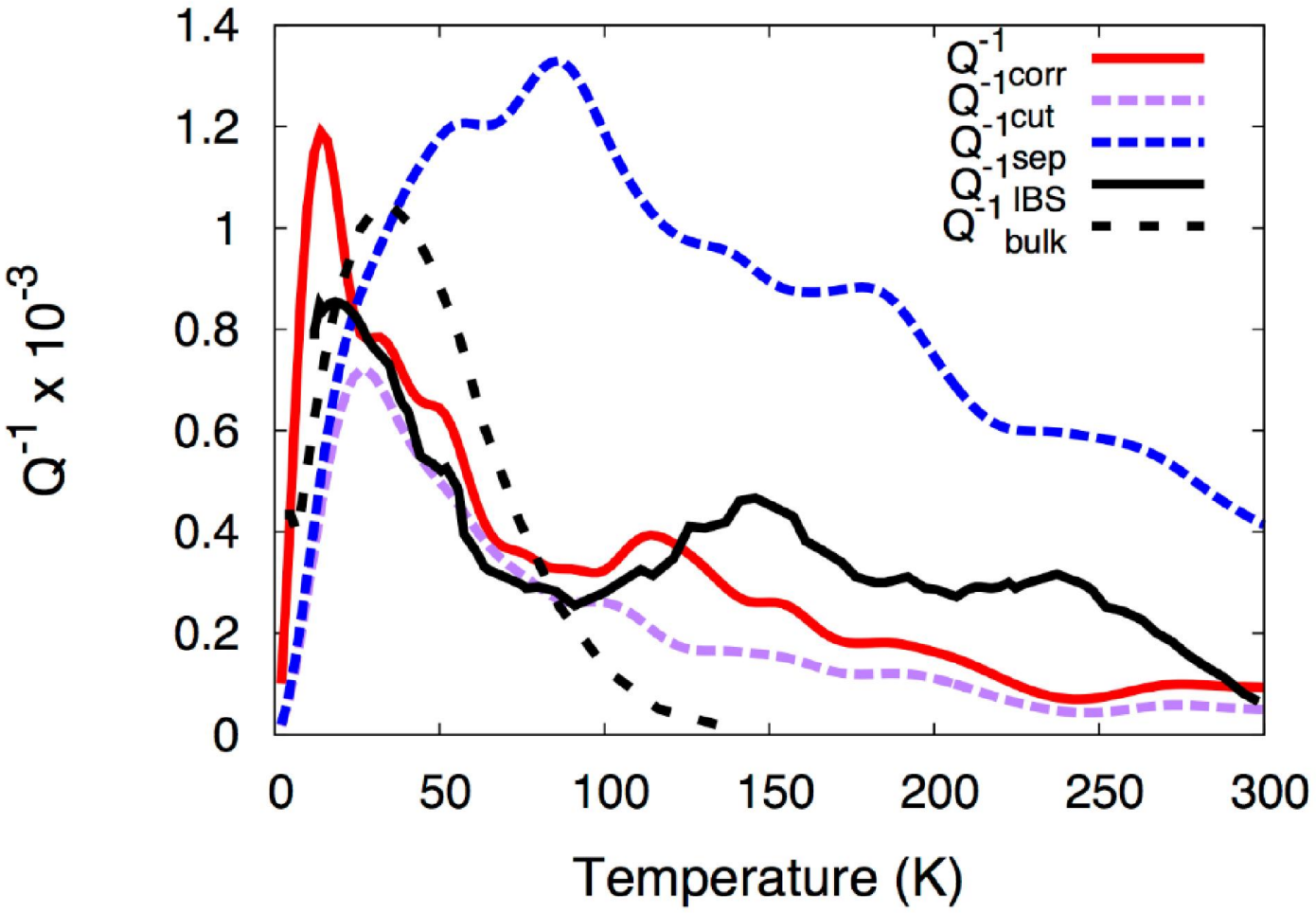
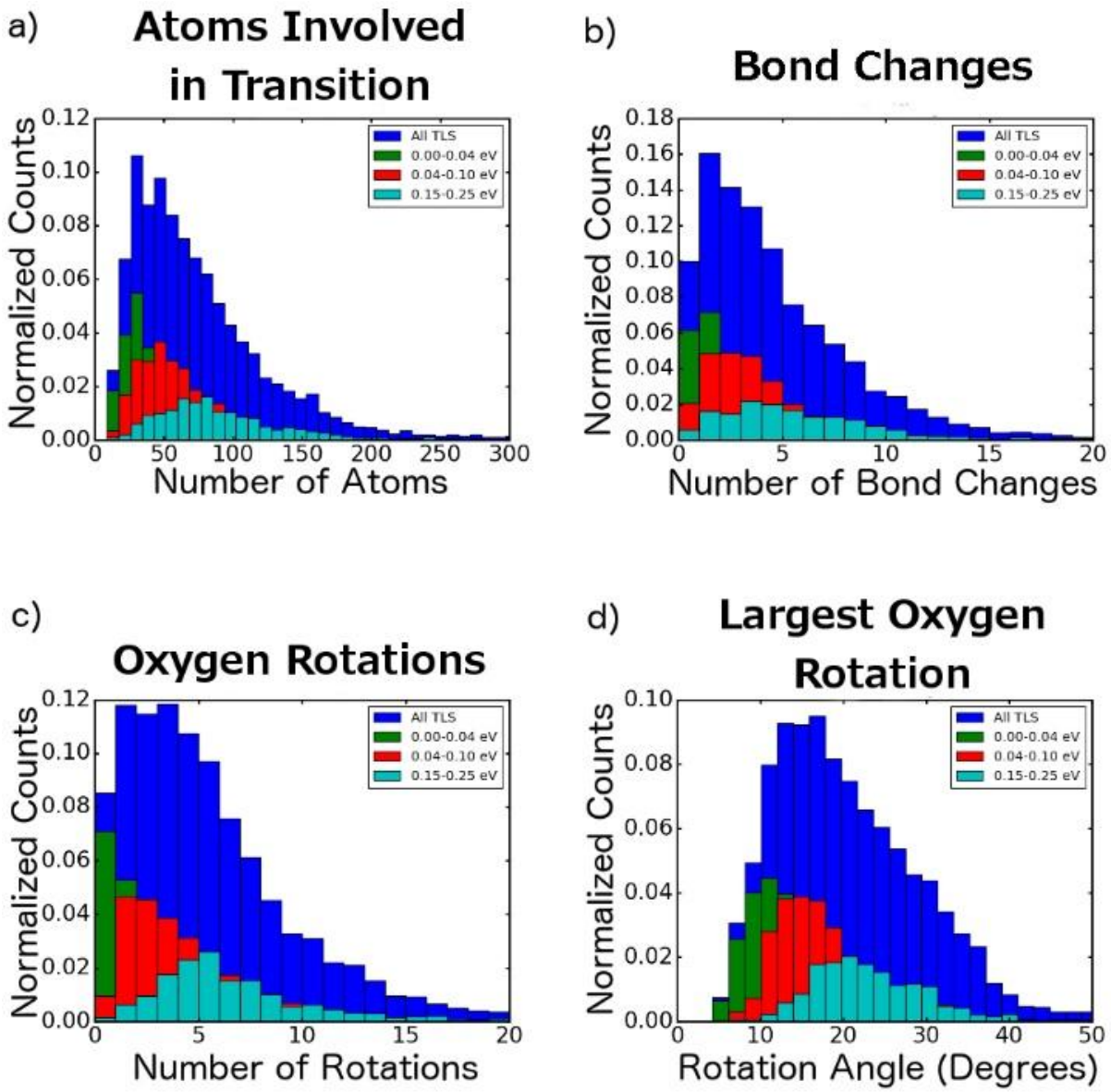
Internal Friction



- $N_{sep}(V, \Delta)$ does not compare well at all to experiment
- $N_{cut}(V, \Delta)$ agrees with low temperature peak
- $N_{corr}(V, \Delta)$ agrees with IBS low temperature peak and second peak around 150K

Statistics of Atomic Transitions



- Features have well-defined distributions
- This suggests the features are due to distinct transitions

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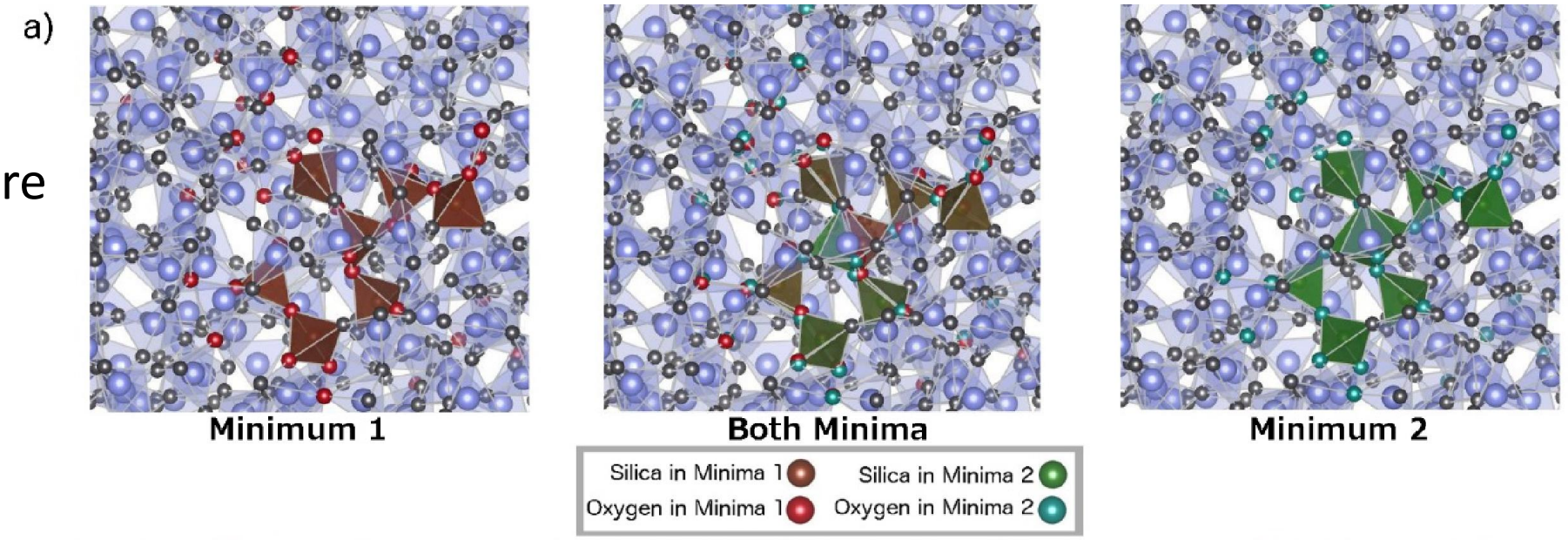
Atomic Transitions

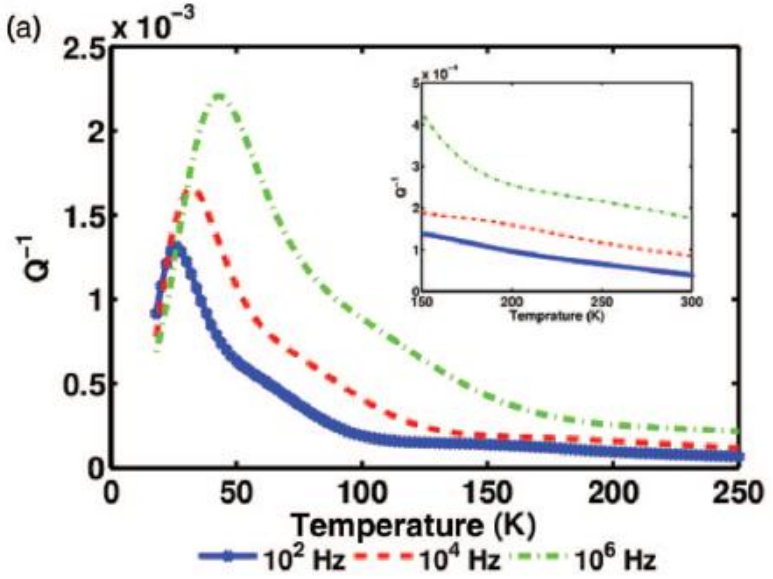
Low Temperature Peak (20 K)

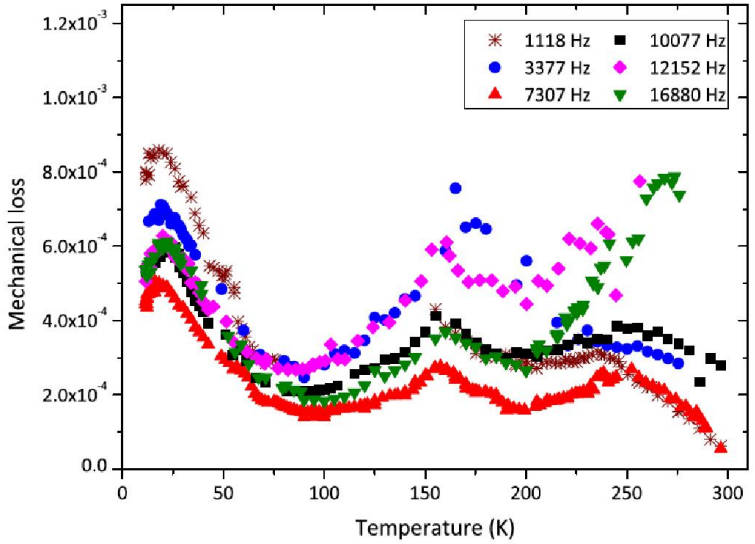


Second Peak (120 K)

Current and Future Work

- New implementation within LAMMPS
  - More options, will improve accuracy of τ_0 and γ
  - More user-friendly interface – facilitates collaboration
- Expanding frequency-dependence of the model, but calculating relaxation time for each TLS
- Density-dependent study of amorphous SiO_2
- Calculating loss of Si-doped tantala and Zr-doped tantala
- Recruited two new students!





3. R. Hamdan, J. P. Trinastic, and H. Cheng, The Journal of chemical physics 141, 054501 (2014).

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Conclusion

- Using classical MD to provide inputs for a TLS model gives good agreement with internal friction measurements in amorphous oxides
- This model allows us to
  - Screen materials by predict effect of doping on the internal friction
  - Understand the atomic transitions that cause internal friction and thermal noise
- The implementation in LAMMPS offers **fast, user-friendly** calculations of the internal friction in amorphous oxides

TLS Distributions

- To facilitate analytical calculations and improve the rate of convergence, previous studies have separated that number density:

$$N_{sep}(V, \Delta) = f(\Delta)g(V)$$

- To improve comparison to experiment, some work also introduces a cut-off for TLS's with Δ above 0.1 eV.

$$N_{cut}(V, \Delta) = f(\Delta)g(V)\Theta(\Delta_{cut} - \Delta)$$

- We compare the results of these two distributions with the correlated distribution, $N_{corr}(V, \Delta)$.

Two-Level System States

- We can diagonalize this Hamiltonian, and we obtain two states with $\pm {}^{E}/_{2} = \pm {}^{1}/_{2}\sqrt{\Delta^2 + \Delta_0^2}$:

$$\psi_1 = \varphi_1 cos\theta + \varphi_2 sin\theta$$
$$\psi_2 = \varphi_1 sin\theta - \varphi_2 cos\theta$$

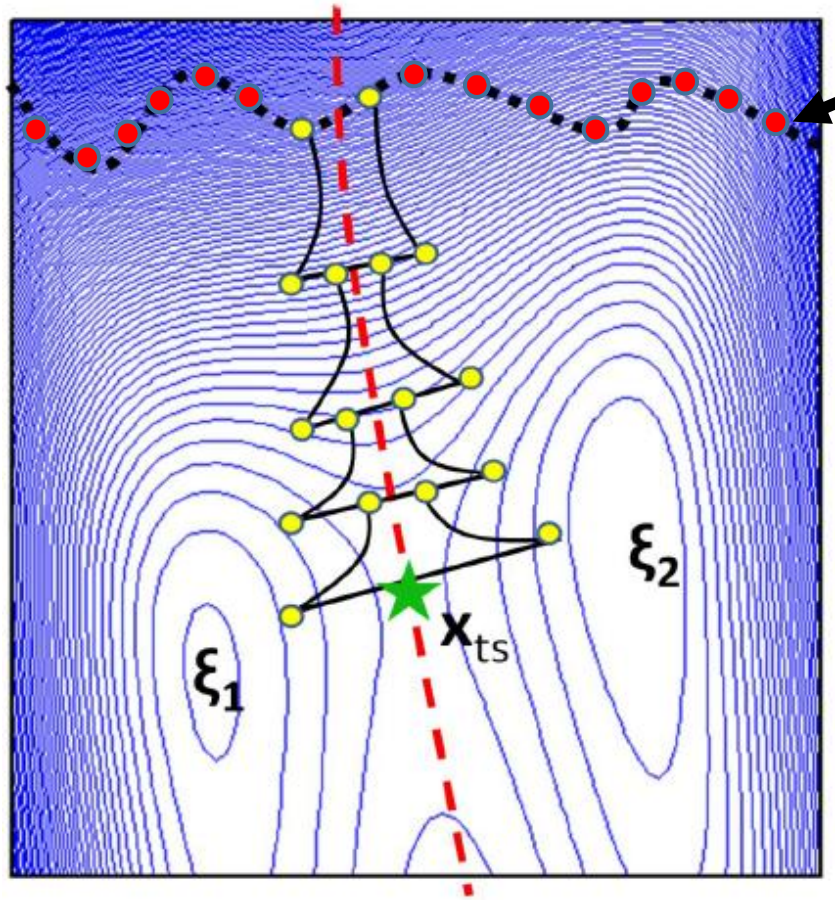
Where $\tan(2\theta) = \frac{\Delta_0}{\Delta}$.

- The dipole moments of each state are

$$p = \pm p_0 \frac{\Delta}{E}$$

where p_0 is the dipole moment of the isolated state ($\Delta \gg \Delta_0$).

The TLS model in MD



Rashid Hamdan, *unpublished*.

- The barrier search moves the system through the potential energy landscape
- This method is repeated tens to hundreds of thousands of times to get a TLS distribution
- The average relaxation time and average coupling constant is calculated from a subset of the discovered TLS's

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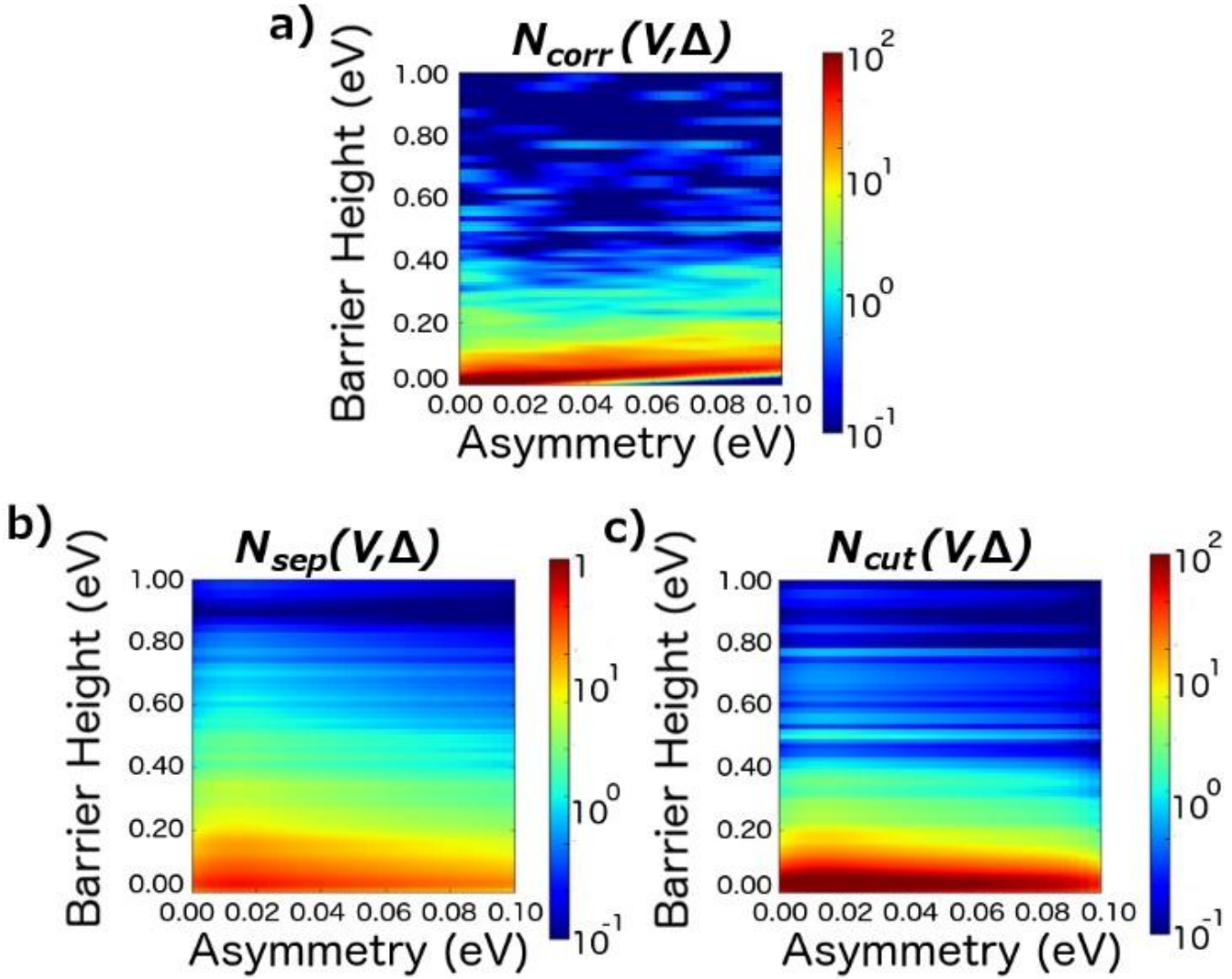
Results: TLS Density



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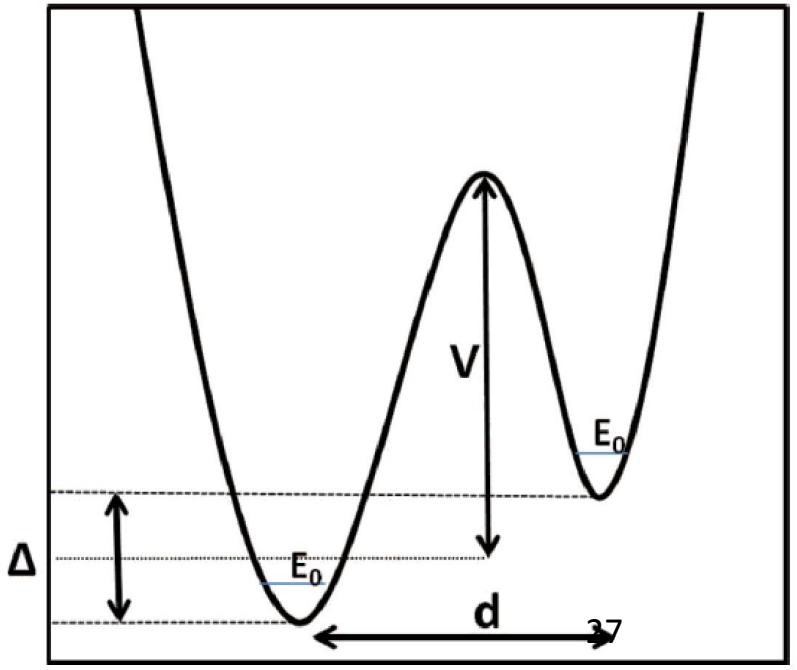
Model Inputs: Elastic Moduli and Coupling

- Young's modulus
  - $\sigma_i = c_{ij}\varepsilon_i$
  - Strain the system to determine what the elastic moduli are
- Coupling Constant
  - $\gamma_j = {}^1/_2 \frac{\partial \Delta}{\partial u_j}$
  - The asymmetry changes as unit cell is strained, which is the coupling to mechanical field.



Model Inputs: Relaxation Time

- The relaxation time is calculated using the Arrhenius law:

$$\tau = \tau_0 e^{\frac{V}{kT}} \mathrm{sech}\left(\frac{\Delta}{2kT}\right)$$

- τ_0 is the inverse attempt frequency. This value is calculated by

$$\tau_0^{-1} = \frac{\prod_{i=1}^{3N} v_i^0}{\prod_{i=1}^{3N} v_i^s} e^{S/k}$$

where v_i^0 and v_i^s are the vibrational frequencies at the minimum and saddle point respectively, and the exponential factor is due to entropy