# Identifying High-Tc transmon candidates with minimal oxide thickness

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# What are transmons?

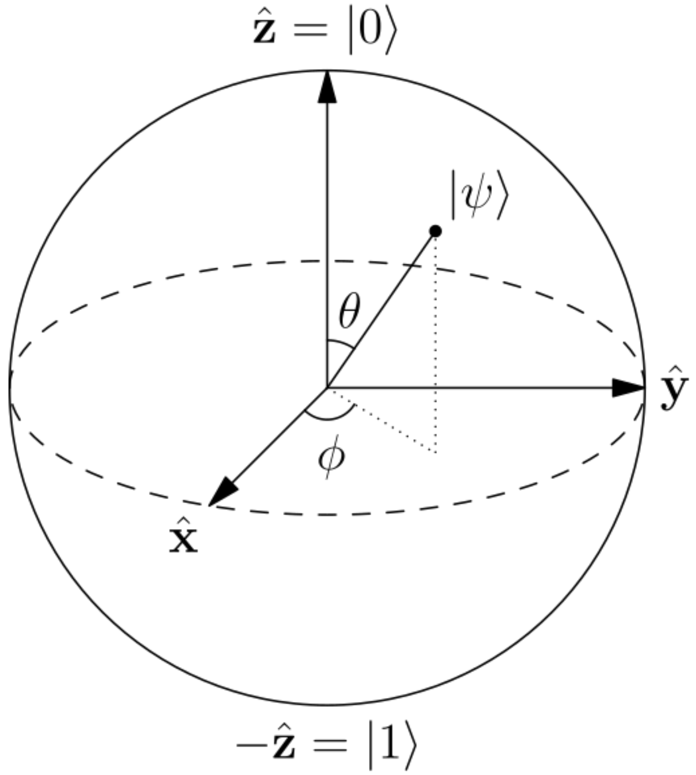
# Quantum Advantage

## Classical bit

0 state

1 state

## Qubit



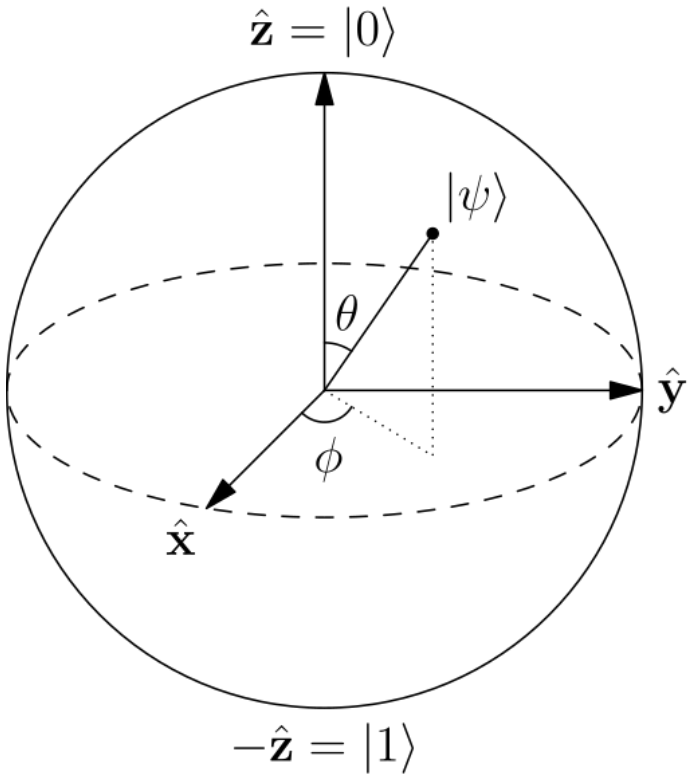

**Probabilistic**
Exact outcome *uncertain* until measurement / interaction

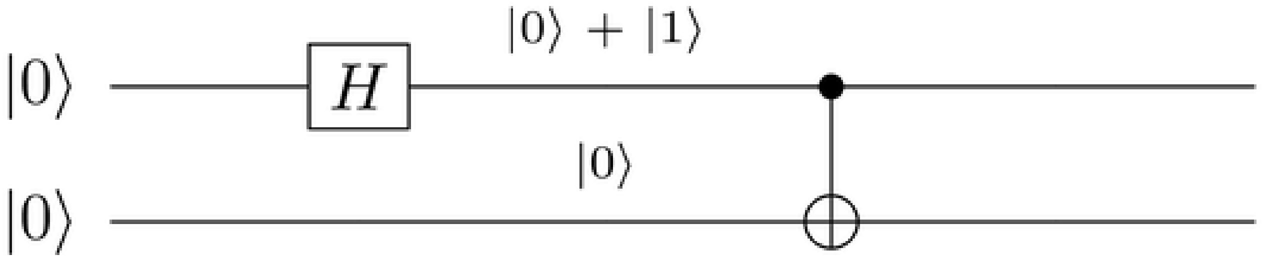
**Entanglement**
Qubit measurement outcomes become correlated after gates

**Quantum tunneling**
**Quantum 'teleportation'**

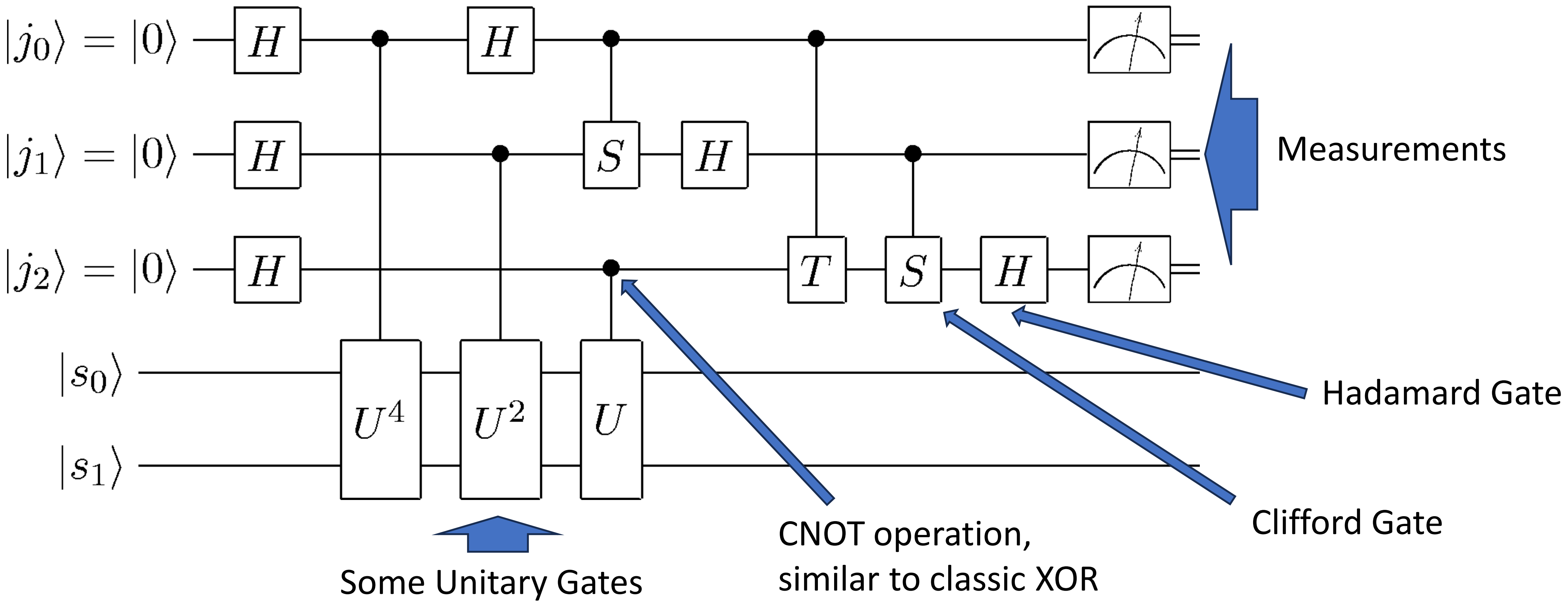
# Quantum Advantage

## Qubit



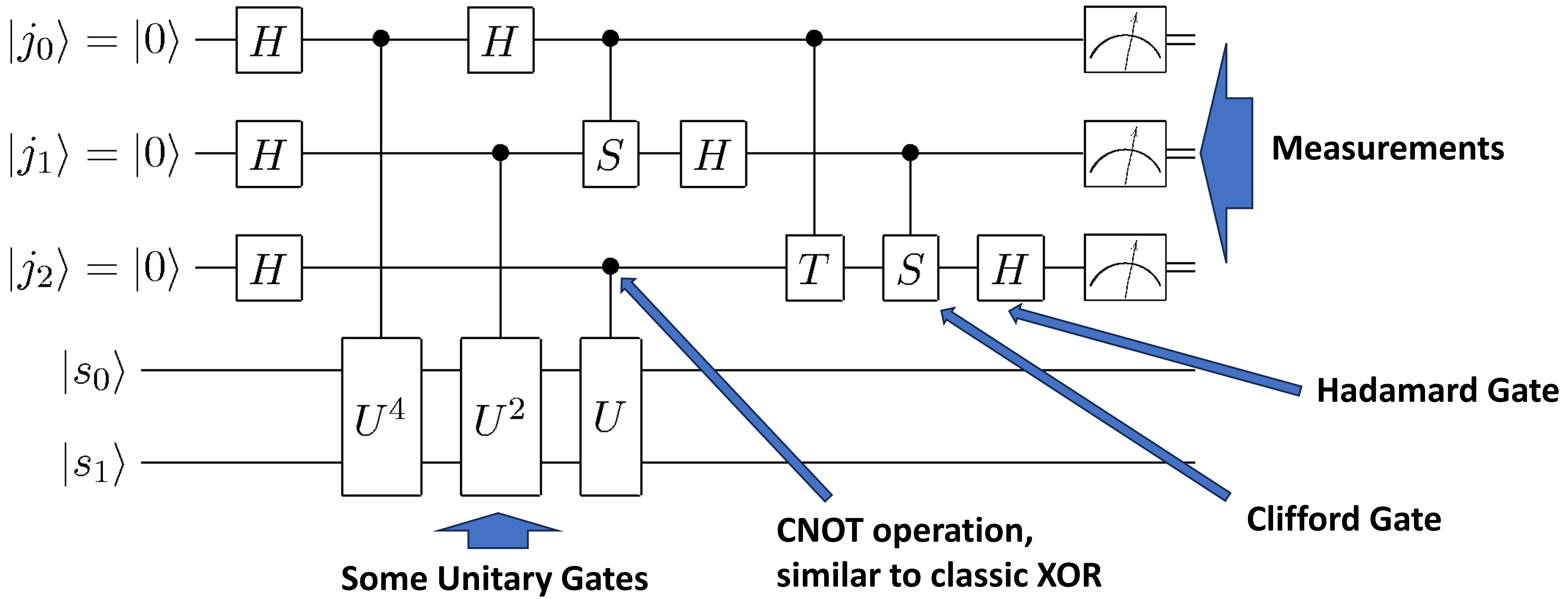




$$\boxed{\frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)}$$




- Highly sensitive to external noise

(insert transitions / arrows while explaining circuit complexity)




- Highly sensitive to external noise

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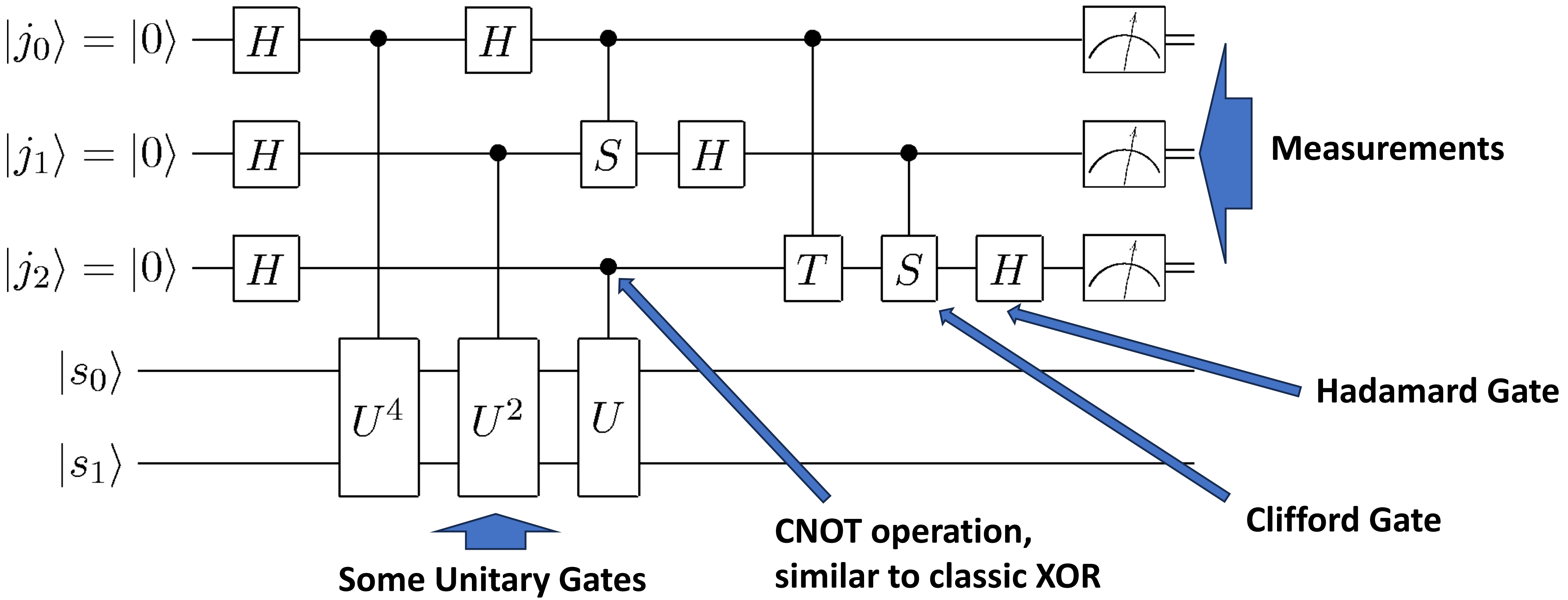



Current record: **0.3 ms, Tantalum**

# Why are oxides important?

# Transmon Decoherence

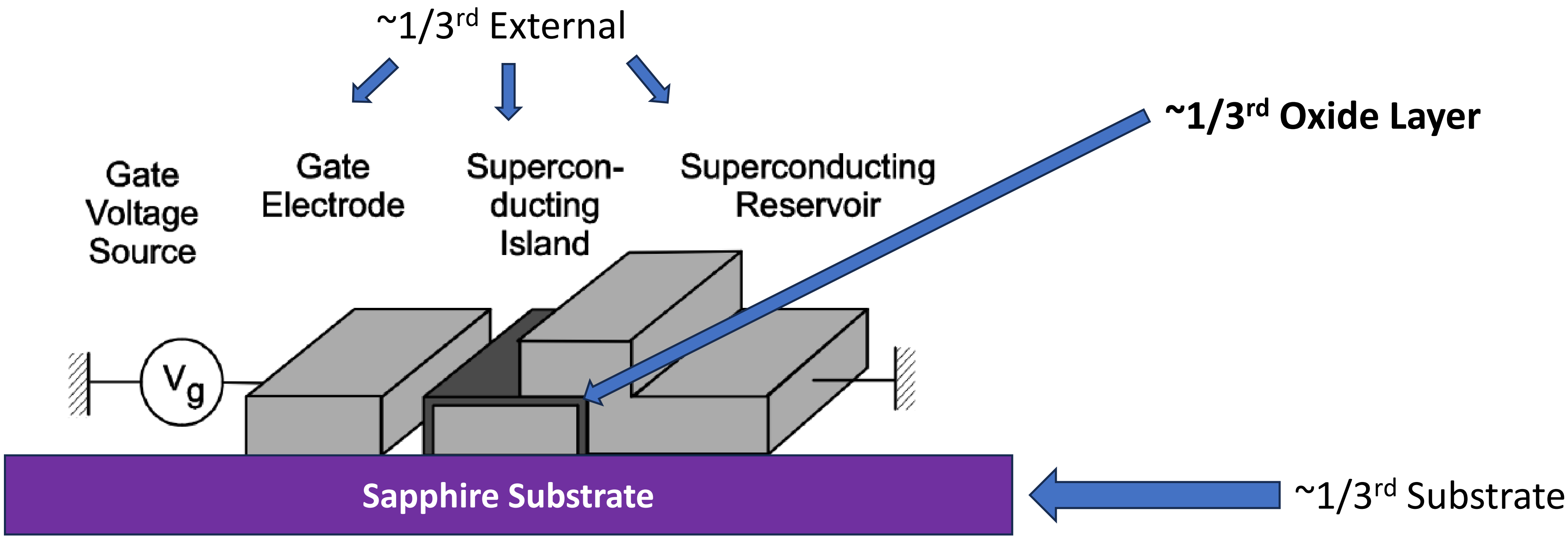
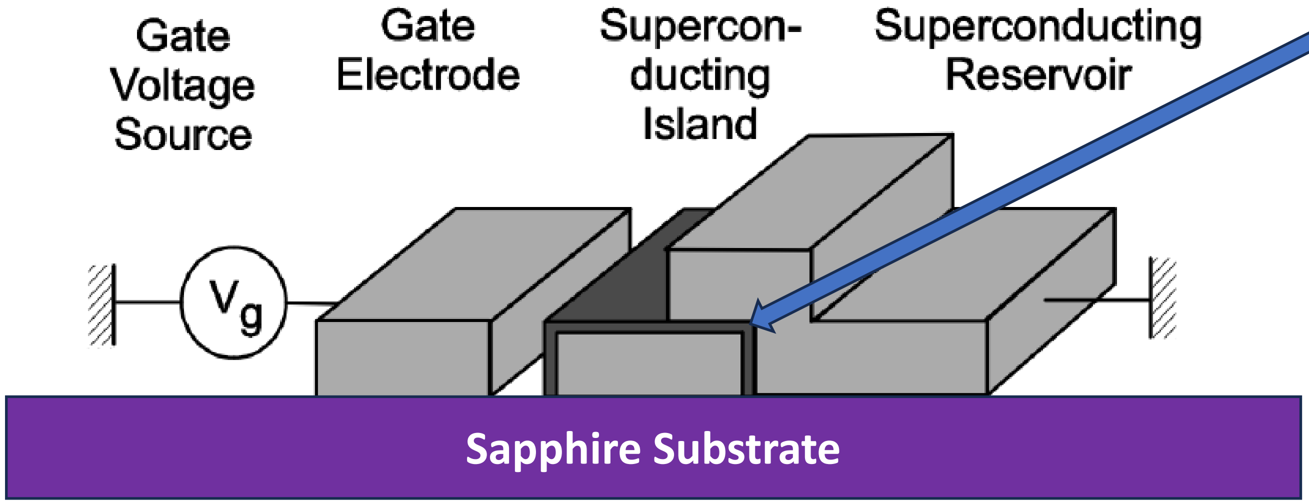



Image Credit: Sam Bader's thesis

Credit: McLellan, Dutta, et. al, Chemical profiles of the oxides on tantalum in state of the art superconducting circuits

# Transmon Decoherence




**~1/3rd Oxide Layer**

- Two-level systems from dangling electrons
- Resonance of microwaves or phonons between oxide layers

Image Credit: Sam Bader's thesis

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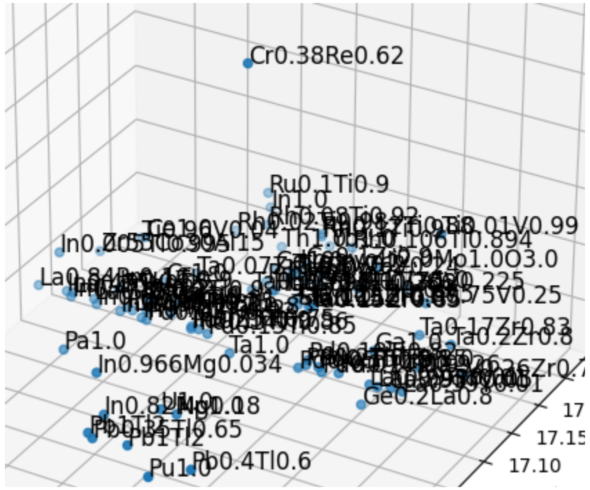
# Developed Metrics

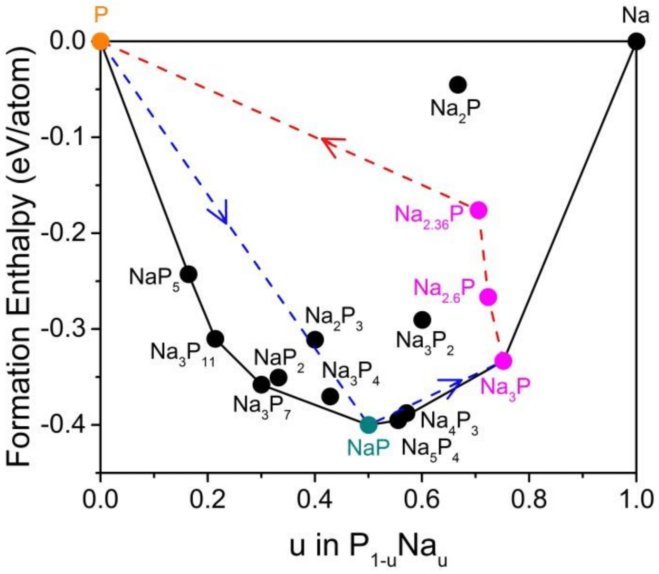
- Oxidation Metric
- % Removable Oxide
- Critical Temperature

# Oxidation Metric

## How likely is a material to form an oxide?




1. Identify potential oxides




2. Solve for minimal energy

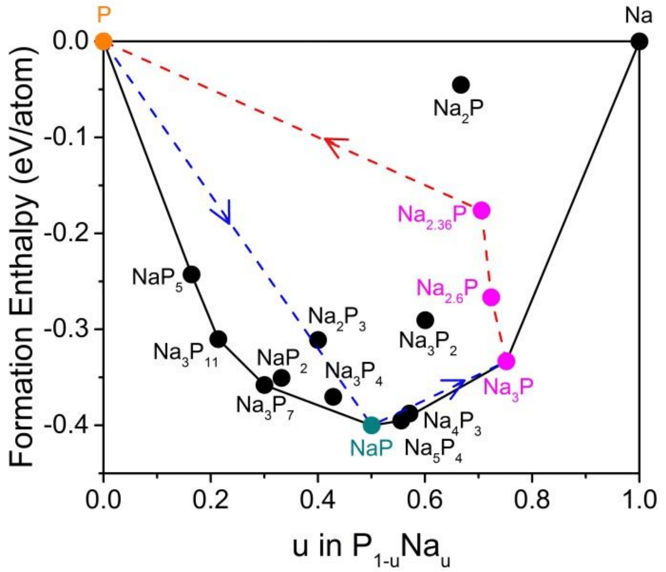
$\Delta H_{Oxides}$ = Net oxide energies
$\Delta H_{Material}$ = Material energy
$\mu = \Delta H_{Oxides} - \Delta H_{Material}$

$$\textit{metric} = \mathbf{1 - \mu / \Delta H_{Oxides}}$$

3. Compare oxide and material Formation Energies

# % Removable Oxide

How much of the oxides could we remove?




2. Solve for minimal energy

**Minimization Data**

- Formation energy of oxide
- Optimal amount oxides

**Additional Data**

- Melting temp of oxides
- Melting temp of material

*Courtesy of ASU's Hong Research Group*

```
for oxide in oxides:
    if oxide_melt < material_melt
        % += oxide_percentage
```

3. Calculate % of removable oxide

# Example: Tantalum

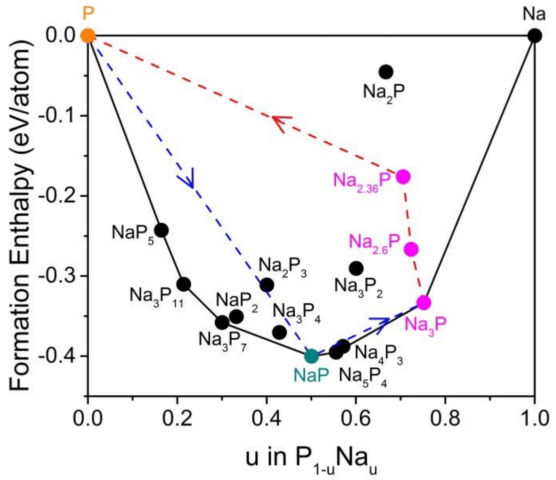
## Identify Ta-based oxides

| Name | Formation E | Features |
|---|---|---|
| Ta2O5 | $\Delta H_{Ta2O5}$ | **Mass** |
| Ta2O3 | $\Delta H_{Ta2O3}$ | **# Atoms** |
| TaO2 | $\Delta H_{TaO2}$ | |
| Ta6O | $\Delta H_{Ta6O}$ | |
| Ta3O8 | $\Delta H_{Ta3O8}$ | |

**Additional Data**

- Melting temp of oxides
- Melting temp of material

*Courtesy of ASU's Hong Research Group*




**ML Model**

Nelder-mead algorithm

**Minimization Goal**

Obtain ideal oxide composition

***Constraints***

- Conservation of mass
- Positivity of material

## Calculate metrics

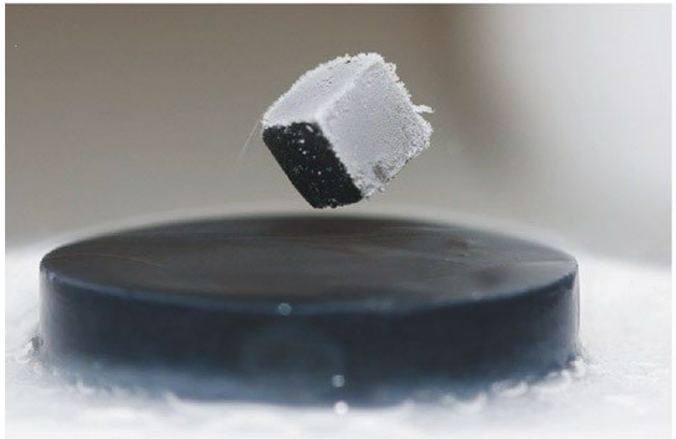
| % Total | Meltable? |
|---|---|
| 55% | No |
| 20% | Yes |
| 10% | No |
| 6% | Yes |
| 9% | No |

**Filler data*

**Net Oxide Formation E**

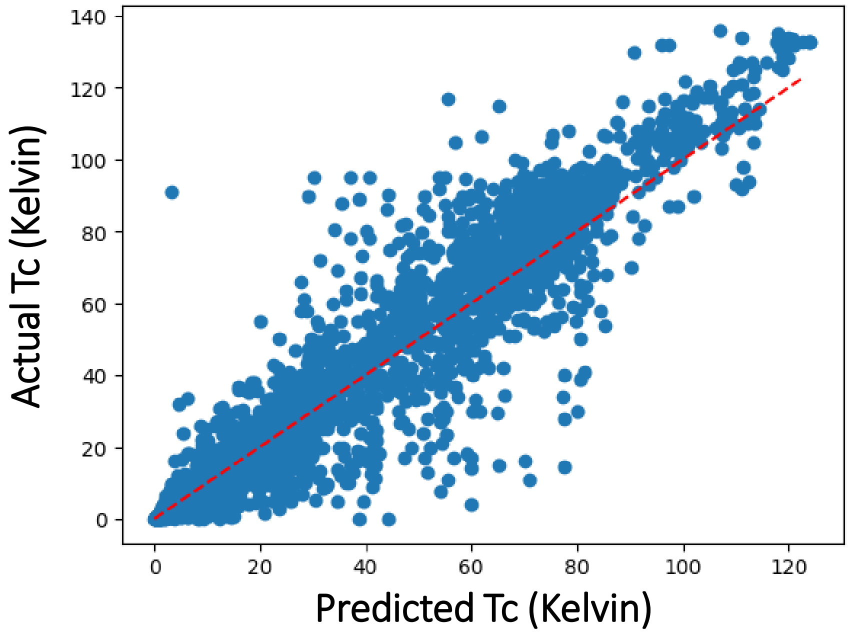
**Net % Meltable Oxide**

# Critical Temperature



1. Take known Tc from SuperCon database

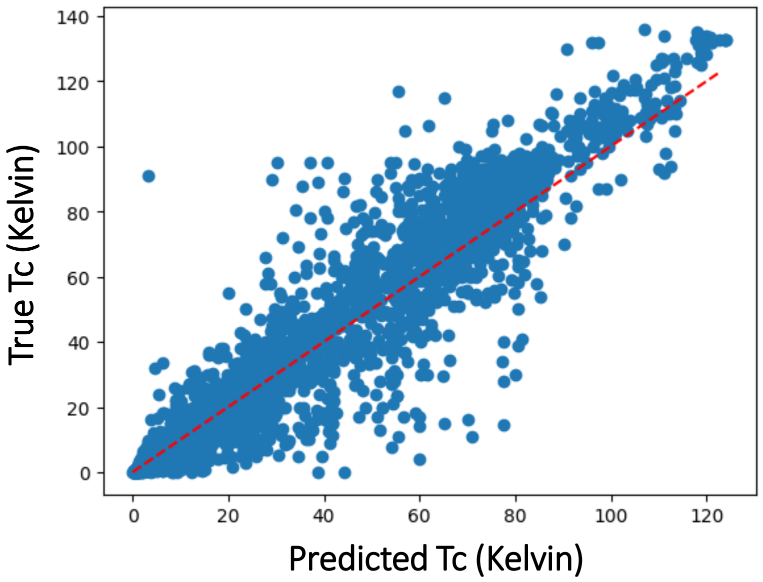
2. Create dataset with elemental composition



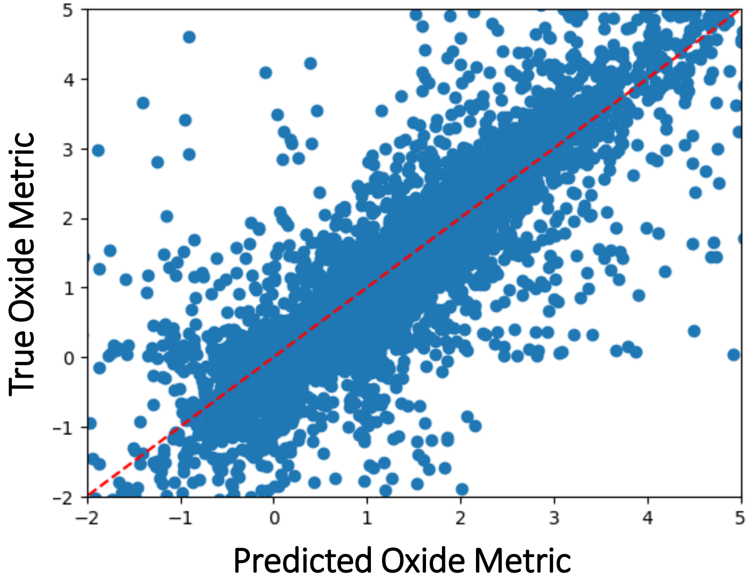

3. Predict Tc for entries from Materials Project

# **Metric Predictability** (w/ **XG boost**)

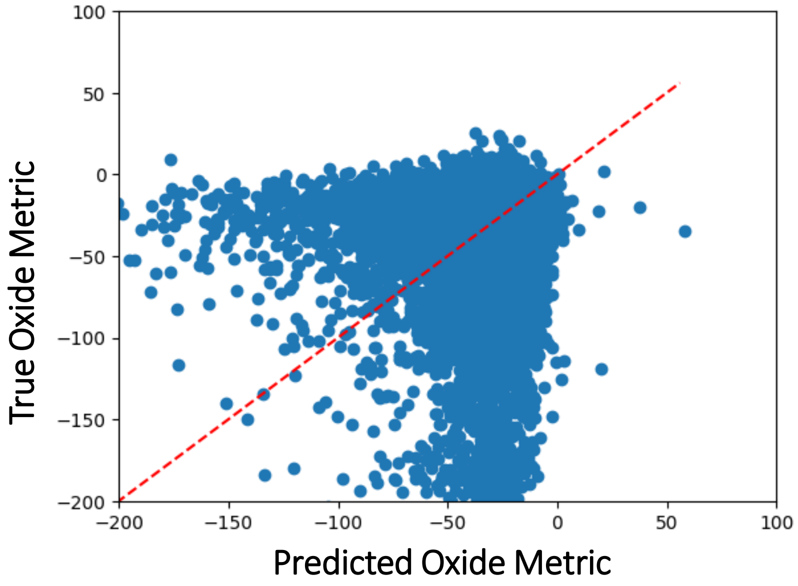
Y-axis: Actual values X-axis: Predicted values




1. Critical Temperature

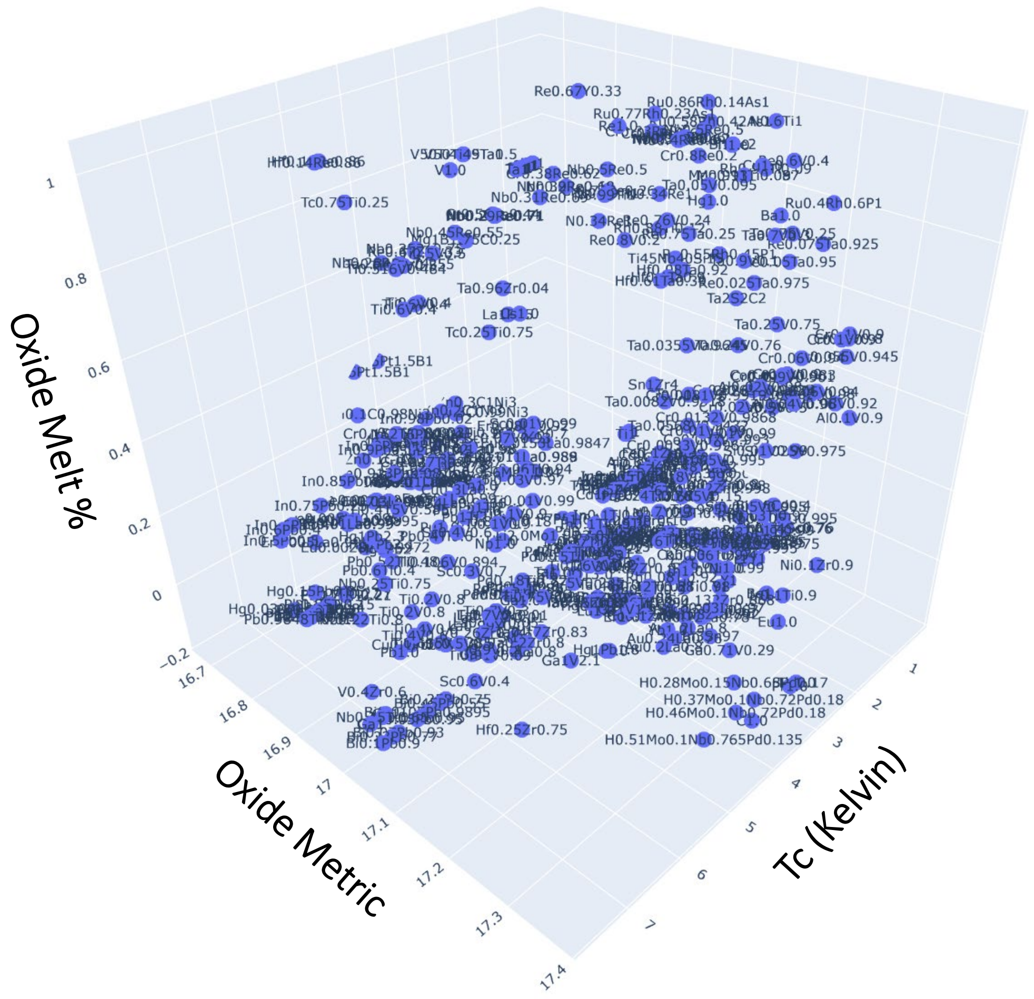



2. Simplified Oxidation Metric




3. True Oxidation Metric

# Material Metrics




## Material Analysis

- Identify material (Ex. Ta, Nb)
- Generate 'neighborhood'
- Identify patterns (Ex. Cuprates)
- Select high-Tc materials with thin oxide layers

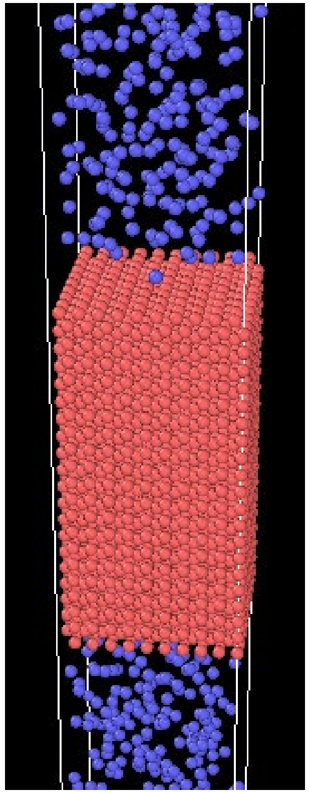
Perform MD simulations for top material candidates

# Results

- Creation of metrics applicable to any material
- Prediction of metrics solely from elemental composition
  - Tc **predictable**, Oxidation Metric **complicated**

# Bonus:

LK-99 'Room-Tc Superconductor' -> `CuP6Pb9O25`
Predicted Tc -> `39.89267 Kelvin`



## Contributors

Tyrel McQueen

## Special Thanks

Jim Overhiser
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McQueen group

JOHNS HOPKINS UNIVERSITY

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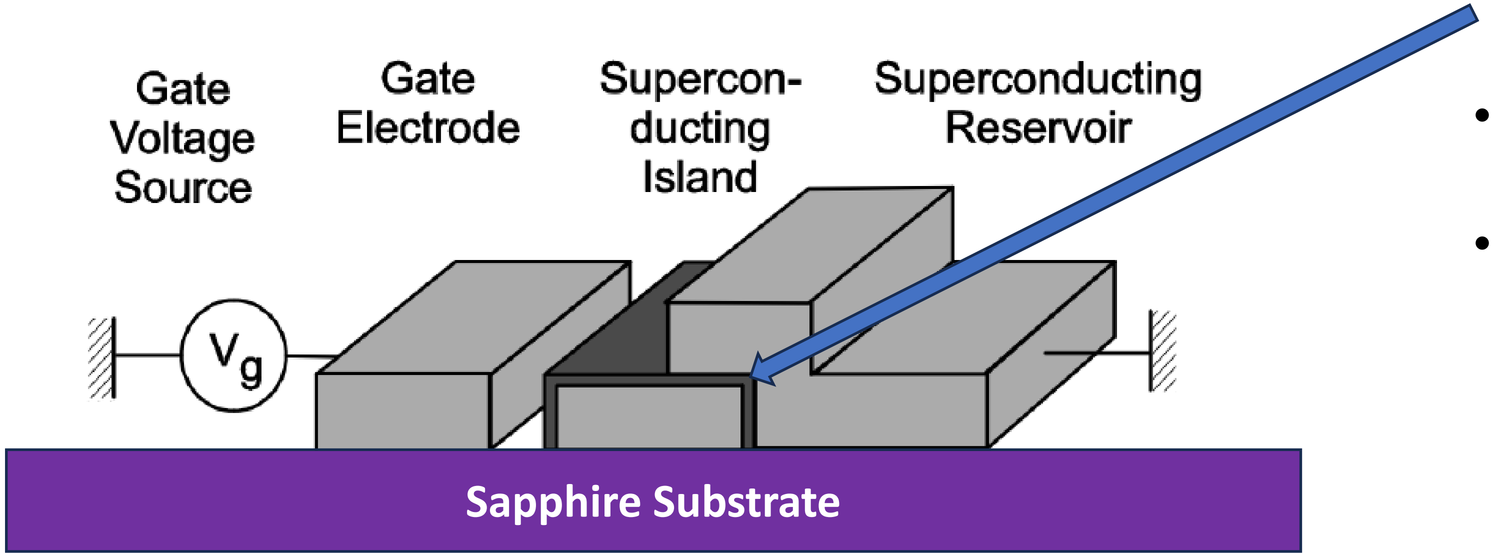
NSF

PARADIM AN NSF MATERIALS INNOVATION PLATFORM

# Bonus+: First-Principles Tantalum Oxidation Simulations

- Force Field calculations for oxide growth
  *(In progress)*

# Transmon Decoherence

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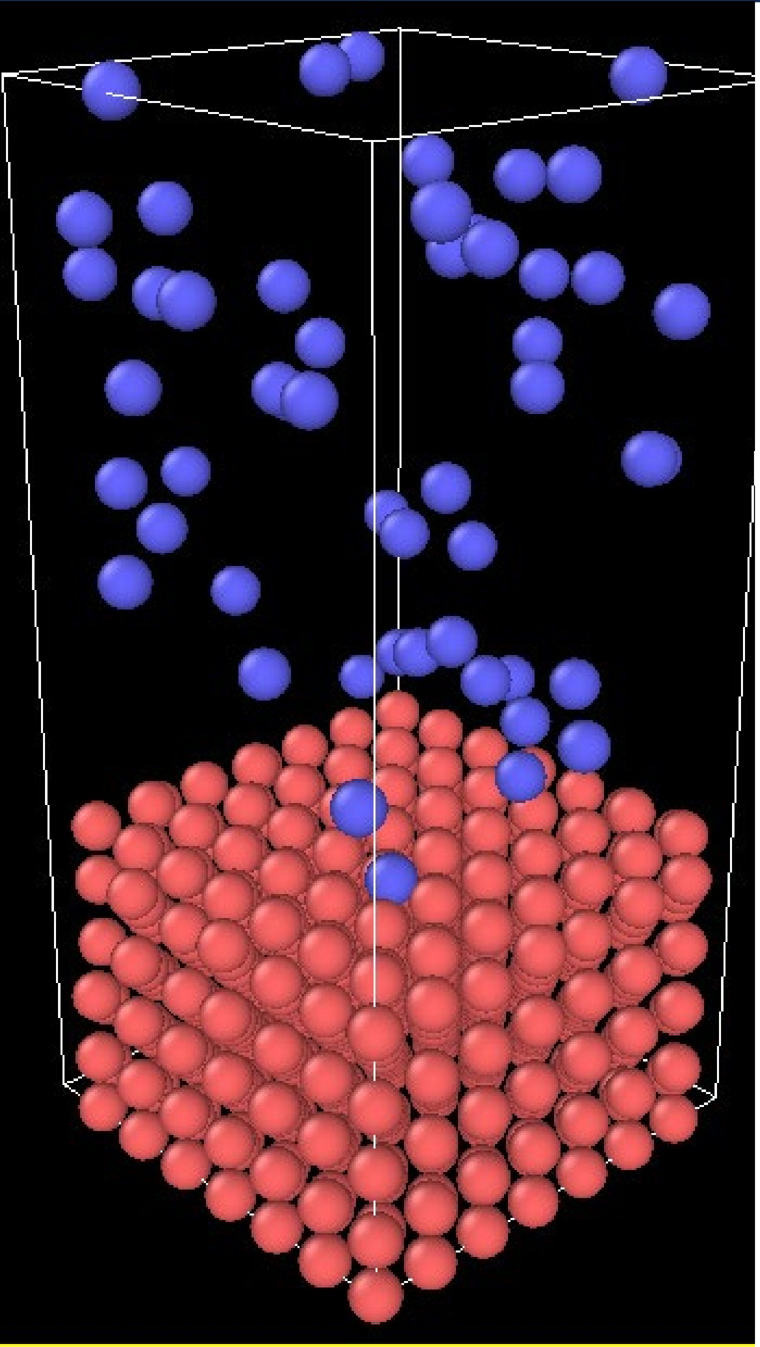


# MD (Molecular Dynamics) for Ta-O interaction

Ta-Ta interaction – PINN potential

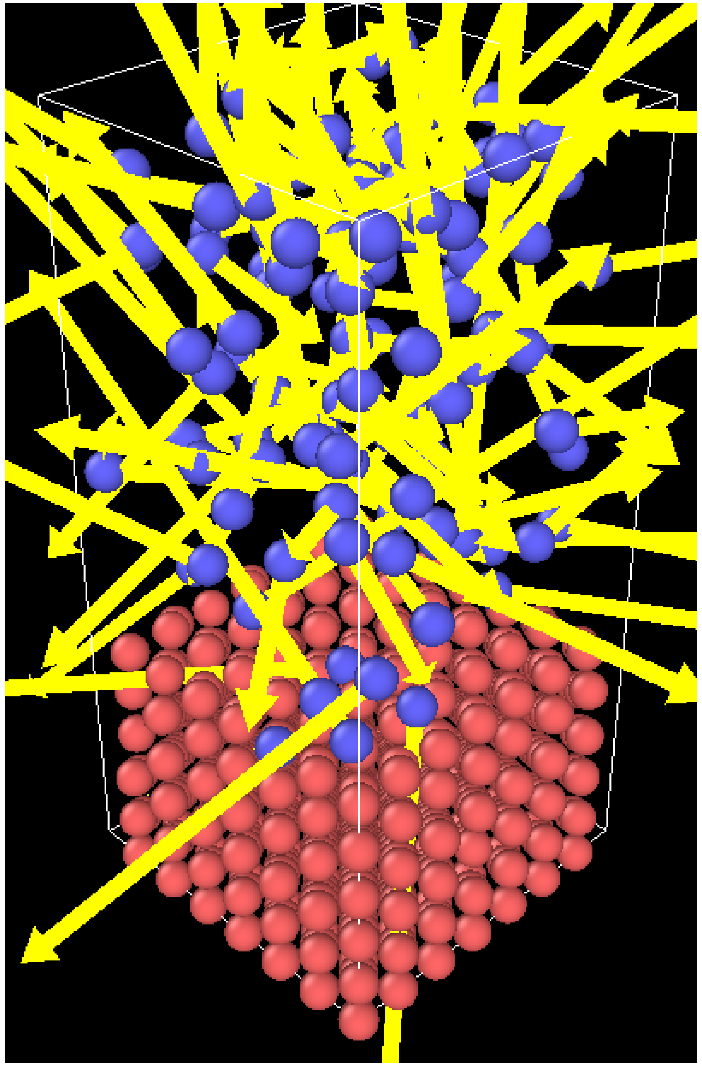
Bonded Ta-O interaction – M-BKS potential

$$\Phi_{ij}^{M-BKS} = q_i q_j / r_{ij} + A_{ij}\exp(-r_{ij}/\rho_{ij}) - C_{ij}/r_{ij}^6 + D_{ij}(1 - \exp(-a_{ij}(r_{ij} - r_e))^2,$$

*In order:*
*Coulomb force, Pauli repulsion, Van-der Waals, Covalent bond (Morse)*

O-O interaction – Lennard-Jones potential

**MISSING:** Non-bonded Ta-O interaction



| Film | $Ta^{5+}$ | $Ta^{3+}$ | $Ta^{1+}$ | $Ta^{0}_{int}$ |
|---|---|---|---|---|
| Native | 2.257 ± 0.023 | 0.370 ± 0.016 | 0.370 ± 0.017 | 0.368 ± 0.019 |
| Ta treated in 10:1 BOE | 1.853 ± 0.028 | 0.296 ± 0.022 | 0.302 ± 0.023 | 0.400 ± 0.021 |
| Ta treated in triacid | 4.826 ± 0.036 | 0.379 ± 0.016 | 0.545 ± 0.020 | 1.198 ± 0.027 |

Current setup:

- Equilibrate system with Nose-Hoover over 5 ps to 300K
- Heating stage with Nose-Hoover over 15 ps to 600K
- Steady temperature for 20 ps

How?

- Minimize oxide layers
- Remove oxides entirely
- **Understand why oxides decohere qubits**

## Why?

- Oxide interfaces have unmatched spin pairs
- Oxide layers cause interference
- Microwave loss amplified by oxide layers

Credit: McLellan, Dutta, et. al, Chemical profiles of the oxides on tantalum in state of the art superconducting circuits