Quantum Simulation of Piezoelectric AlN Alloys Using Pasqal's Pulser

Project Objective: Quantum Simulation of Piezoelectric Materials for Energy Harvesting

Objective: Leverage Pasqal's Pulser platform to simulate and optimize Aluminum Nitride (AlN)-based piezoelectric materials, exploring alloying (e.g., with CrN) and doping to enhance piezoelectric coefficients (e33, d33) and elastic constants (C33) for improved energy harvesting.

by Hugo Cristian Ojeda

Project Context

1 AlN's wurtzite structure

Offers inherent piezoelectricity (d33 ≈ 5.5 pC/N)

2 Alloying potential

CrN increases d33 4x

3 Application areas

Can boost performance for sensors and energy devices

Context: AlN's wurtzite structure offers inherent piezoelectricity (d33 ≈ 5.5 pC/N), but alloying (e.g., CrN increases d33 4x) can boost performance for sensors and energy devices.

Made with Gamma

Phase 1: Compute Hamiltonian and Piezoelectric Coefficients

1

Objective

Develop and simulate a Hamiltonian for piezoelectric AlN using Pasqal's quantum simulation platform (Pulser) to compute a realistic ground state energy and extract key piezoelectric coefficients (e33, d33, C33).

2

Approach

Use Variational Quantum Eigensolver (VQE) with a Stillinger-Weber (SW) two-body potential to model AlN's lattice dynamics (phonons) via qubit-encoded displacements (e.g., ±0.01 Å). Target a ground state energy of −8 to −16 eV for a 16-atom cluster, validated against DFT benchmarks.

3

Outcome

Obtain baseline piezoelectric properties (e.g., e33 ≈ 1.5 C/m2, C33 ≈ 395 GPa) as a foundation for material optimization.

Made with Gamma

Phase 2: Alloying AlN for Enhanced Properties

1

Objective

Combine alloying (e.g., CrN) with AlN to enhance piezoelectric properties for energy harvesting, using DFT-informed algorithms simulated on Pulser to predict and optimize material performance.

2

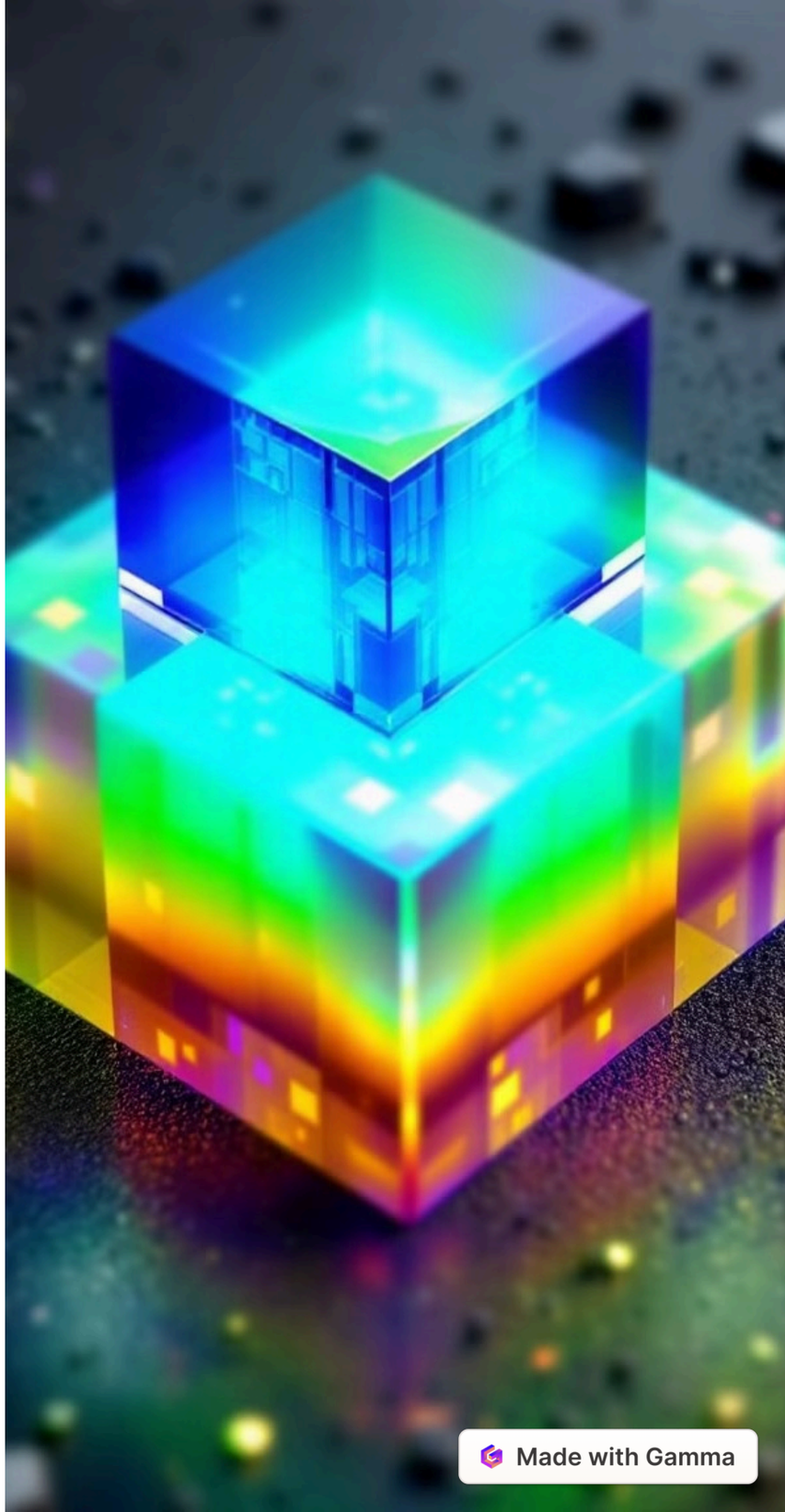
Approach

Modify the Hamiltonian to include alloying effects (e.g., Cr-N pair potentials), leveraging DFT data to simulate changes in energy and coefficients. Use Pulser's scalability to test multiple alloying/doping scenarios (e.g., Cr, Sc, Yb).

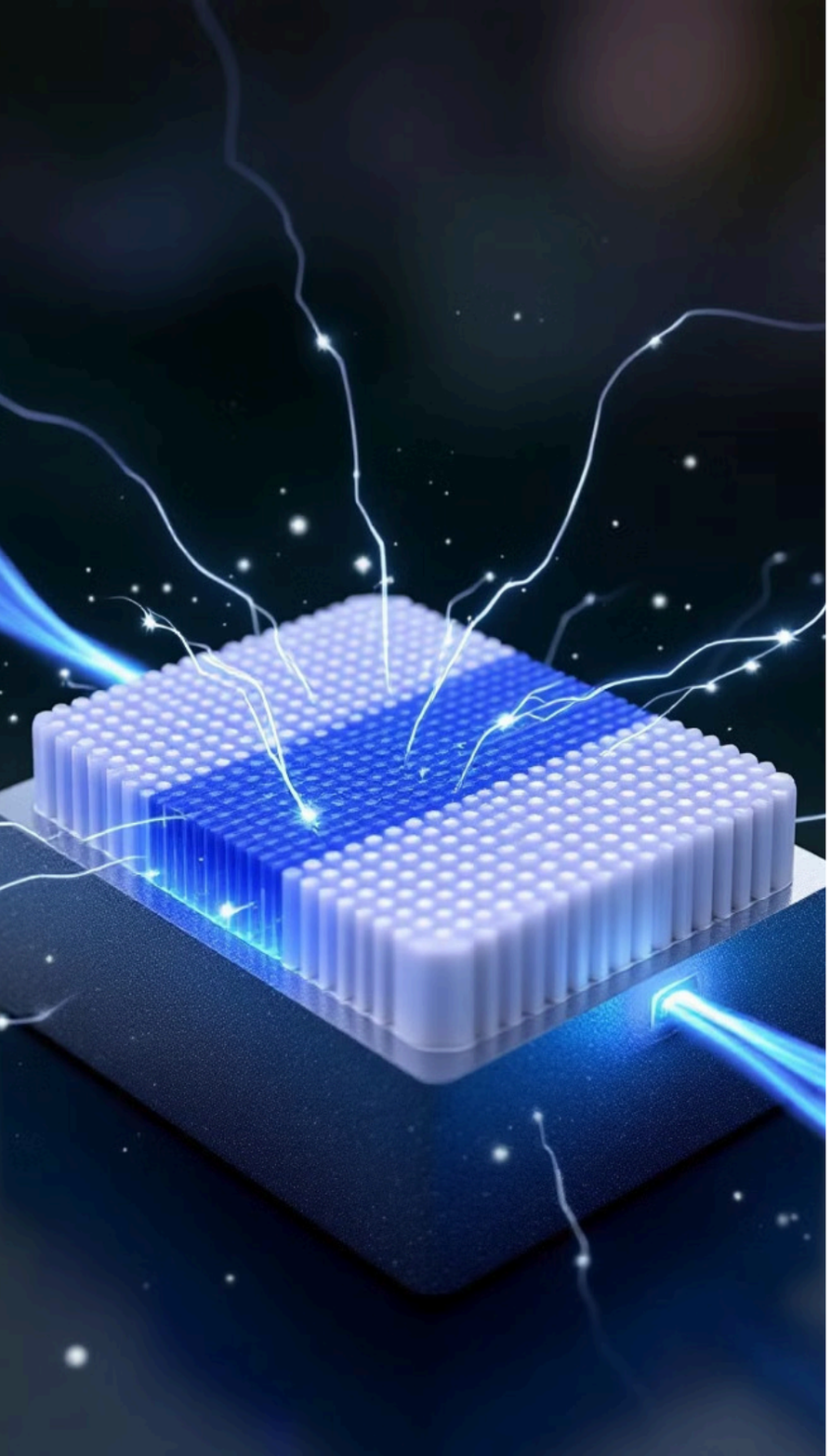
3

Outcome

Identify AlN alloys with improved d33 (e.g., > 22 pC/N) and energy harvesting efficiency, validated against DFT and experimental benchmarks.



Made with Gamma



Goals of the Algorithm

Accurate Ground State Energy

−8 to −16 eV for a 16-atom AlN cluster (Phase 1)

Lattice Dynamics

Simulate phonon-like vibrations for piezoelectric response (Phase 1)

Piezoelectric Properties

Estimate e33, C33, d33 under strain (Phase 1)

Alloying/Doping Effects

Predict enhancements in d33 with new AlN-based materials (Phase 2)

Outcome: A quantum framework to screen AlN alloys/dopants for superior energy harvesting efficiency.

Made with Gamma

Code Explanation (Pulser Simulation)

Overview

Uses Pulser's VQE to simulate a 16-qubit AlN cluster, targeting ground state energy.

Key Components

- Register: 16 qubits in a 4x4 grid (4 μm spacing), encoding displacements (±0.01 Å)
- Hamiltonian: SW two-body potential over 16 nearest-neighbor pairs, scaled to μm units with a mapping to Å
- VQE: Two-layer pulse sequence (52 ns), optimizing energy over 1000 samples with debugging outputs
- Visualization: register.draw() and seq final.draw() for structure and pulses
- Execution: Computes energy iteratively, aiming for −8 to −12 eV

Made with Gamma

Hamiltonian for Piezoelectric AlN

1

Hamiltonian Design

Simplified Stillinger-Weber (SW) Two-Body Potential

2

Form

$$H = \sum_{(i,j)\in \text{pairs}} V_2(r_{ij}),$$

$$V_2(r_{ij}) = A\epsilon \left[B \left(\frac{\sigma}{r_{ij}} \right)^p - \left(\frac{\sigma}{r_{ij}} \right)^q \right] \exp\left(\frac{\sigma}{r_{ij} - r_{\text{cut}}} \right).$$

3

Parameters

ϵ = 0.8 eV, σ = 1.9 Å, rcut = 3.0 Å, A = 7.05, B = 0.60, p = 4, q = 0

Physical Relevance:

- Phonon Representation: Displacements (±0.01 Å) mimic lattice vibrations, scaled from 4 μm to 1.9 Å via a factor (1.9/4.0)
- Bonding Energy: Each pair −0.5 to −1 eV, targeting −8 to −12 eV for 16 atoms
- Piezoelectric Basis: Foundation for adding strain-polarization coupling later

Implementation: Maps μm distances to Å-scale potential, summing over 16 pairs.

Made with Gamma

Advantages of Quantum Computing with Pasqal & Next Steps

Why Pasqal?

- Scalability: 16 qubits now, expandable to 32+, vs. DFT's small-cell limits
- Flexible Interactions: Rydberg couplings mimic dipole effects for polarization
- Quantum Optimization: VQE speeds up ground state searches for alloys/dopants
- Direct Simulation: Qubit displacements model phonons natively

Advantages for Discovery

- Alloying/Doping: Predict CrN or ScN effects (e.g., d33 > 22 pC/N)
- Energy Harvesting: Optimize C33, e33 for efficiency
- Speed: Faster screening vs. classical DFT

Summary: Phase 1 simulates AlN's ground state (−8 to −12 eV), setting up Phase 2 to enhance properties via alloying with Pulser and DFT algorithms.

Next Steps:

- Add three-body and coupling terms for full piezoelectricity (Phase 1 continuation)
- Expand to 32 qubits and test CrN/Sc doping (Phase 2)

Made with Gamma