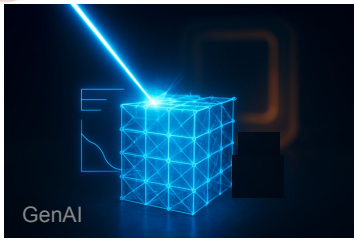
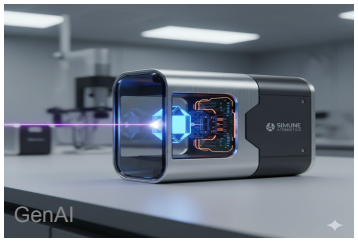
# Predictive Modeling for High Energy Sensing

## Accelerating Detector Design via Electronic Structure Modeling




### The Challenge:

**Trial-and-Error**: Balancing light output and decay time via slow, costly physical synthesis.

**Empirical Design:** Tuning luminescence without precise quantum data on electronic band structures

### The Solution:

**Electronic Mapping:** Uses DFT (SIESTA/QE) to extract energy levels governing light emission.

**Dopant Analysis:** Predicts exact impurity levels and defect formation

### Strategic Impact:

- **Virtual Screening**
- **Performance Optimisation**
- **Reduced Development Cost**

# The Challenge

**Scintillator Crystals** (used in medical imaging, security, and physics experiments) must be **highly efficient at absorbing high-energy radiation** (X-rays or γ-rays) and **re-emitting it quickly as visible light.**

Optimizing materials requires balancing three competing factors (Light Output, Decay Time, and Cost). Traditional trial-and-error synthesis is slow and costly.

Without precise **quantum mechanical data on the electronic band structure,** developing new dopant chemistries to tune luminescence is a trial-and-error process.

# The Solution

**ASAP (Atomistic Simulation Advanced Platform)**

A single, integrated platform utilizing DFT methodology (SIESTA and Quantum Espresso codes) to extract critical physical data. ASAP precisely calculates the electronic energy levels that govern light emission.

Characteristics computed:

- Band Structure
- Density of States (DOS)
- Defect Formation Energies

# Core Insight: Electronic Structure

**Electronic Structure** (Band Gap, DOS, and Impurity Levels) dictates the color, intensity, and speed of the emitted light (Luminescence).

ASAP **predicts the exact energy levels** introduced by dopant atoms (like $Ce^{3+}$ or $Eu^{2+}$) or defects, which act as the scintillation centers.

# Impact

**Quantum-Accelerated Discovery for Optimal Scintillators**

- **Accelerated Discovery**: Enables the virtual screening of potential halide or oxide crystal compositions (and dopant combinations) to identify candidates that meet specific performance criteria (e.g., maximizing efficiency).

- **Reduced Development Cost**: Replaces expensive, slow synthesis and physical characterization with rapid, high-throughput computational screening.

- **Performance Optimization**: Provides the data required to fine-tune the material's properties, predicting the correct dopant concentration needed to maximize scintillation speed and yield.

# Technical Validation: Publications

These publications validate the DFT methodology (SIESTA code) for calculating Electronic Structure and Optical Response. ASAP simplifies and accelerates this exact analysis.

- Crystal growth, structural and electronic characterizations of zero-dimensional metal halide (TEP)InBr4 single crystals for X-ray detection

- Phase Transitions in Low-Dimensional Layered Double Perovskites: The Role of the Organic Moieties

- Halide Mixing in Cs2AgBi(IxBr1–x)6 Double Perovskites: A Pathway to Tunable Excitonic Propertie

- Crystal growth, structural and electronic characterizations of zero-dimensional metal halide (TEP)InBr4 single crystals for X-ray detection

# Next Steps: Start Your Atomistic Simulation

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**Schedule a Free Strategic Consultation:** Discuss your material challenge with our scientific team

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