

Predictive Modeling for High Energy Sensing: Scintillators

Accelerating Detector Design via Electronic Structure Modeling



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.

Developing new dopant chemistries to tune luminescence is speculative without precise **quantum mechanical data on the electronic band structure**

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.

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.

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\(IxBr_{1-x}\)₆ Double Perovskites: A Pathway to Tunable Excitonic Properties](#)
- [Crystal growth, structural and electronic characterizations of zero-dimensional metal halide \(TEP\)InBr₄ single crystals for X-ray detection](#)



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