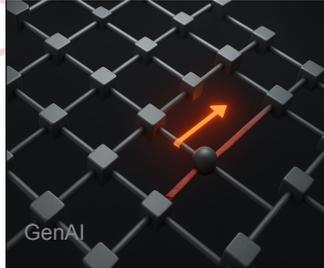


Threshold Displacement Energy Mapping



The Challenge:

Materials in nuclear, satellite, and particle environments degrade under constant high-energy particle bombardment. **Predicting structural longevity** is critical for safety, yet traditional models lack the quantum-accurate parameters to forecast failures



The Solution:

Molecular Dynamics workflow to execute quantum-accurate "collision experiments" on individual atoms: **Threshold Displacement Energy (E_d)**



Strategic Impact:

- **Virtual Screening**
- **Process Guidance**
- **Accelerated Qualification**

Irradiation-Critical Materials in advanced nuclear reactors, satellites, and particle accelerators are **degraded by constant high-energy particle bombardment**. Predicting how long a structural component (like a steel alloy or SiC ceramic) will last is vital for safety, yet traditional models are fundamentally flawed.

Industry-standard simulation tools rely on average, often inaccurate, Threshold Displacement Energy (E_d) values derived from decades-old data.

Unreliable long-term damage prediction, leading to conservative designs, increased costs, and risk of premature component failure.

ASAP (Atomistic Simulation Advanced Platform)

A single, integrated platform utilizing DFT methodology (SIESTA and Quantum Espresso codes) to extract critical physical data

- ASAP's Molecular Dynamics workflow to execute quantum-accurate "collision experiments" on individual atoms.

Characteristics computed:

- Threshold Displacement Energy (E_d)

The **Threshold Displacement Energy** (E_d) is the minimum energy required to permanently knock an atom out of place, creating a damaging defect.

This directional E_d mapping finds the material's weak spots, the crystal directions most susceptible to damage, which are often missed by bulk experiments.

Quantum Modeling with ASAP:

Using the ASAP Molecular Dynamics Workflow, you can initiate a displacement event by giving a Primary Knock-on Atom (PKA) a precise kinetic energy, and then monitor the system's full quantum-mechanical response over picoseconds.

Ed-Driven Material Qualification

- **Virtual Screening:** Enables the virtual screening of complex new alloys and ceramics for inherent radiation hardness before expensive prototypes are manufactured.
- **Process Guidance:** Guides manufacturing processes by identifying how component orientation relative to expected particle flux impacts lifetime.
- **Accelerated Qualification:** Provides the most accurate, directionally-resolved Ed values to feed into macro-scale transport and damage codes.

These publications validate the DFT methodology (SIESTA code). ASAP automates the required SIESTA calculations for rapid R&D application.

- [Electronic energy loss and damage efficiency in ceramics under ion irradiation: Insights from first-principles simulations](#)
- [Ab initio molecular dynamics investigation of threshold displacement energies and defect production in Gd₂Ti₂O₇ pyrochlor](#)
- [Threshold Displacement Energies in Lead Halide Perovskites from Ab Initio Molecular Dynamics Simulations](#)
- [Ab initio molecular dynamics simulations of defect generation and thermal stability in 3C-SiC](#)
- [Ab initio molecular dynamics simulations of low-energy recoil events in ThO₂, CeO₂, and ZrO₂](#)

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

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The main logo for SIMUNE ATOMISTICS. The word 'SIMUNE' is rendered in a large, bold, sans-serif font with a vertical color gradient from orange at the bottom to red at the top. The letter 'S' is uniquely designed, with its upper portion forming a molecular structure of red and white spheres connected by lines. Below 'SIMUNE', the word 'ATOMISTICS' is written in a smaller, grey, all-caps, sans-serif font with wide letter spacing.

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