Predictive Modeling for Fusion/Fission Reactors

Simulating the formation energies, migration barriers, and interaction of radiation-induced defects

The Challenge

Materials crucial for **extreme environments,** such as Steels, Tungsten and SiC, are fundamentally limited by **aging**. Defects created by radiation do not sit still; they migrate and cluster over years, leading to catastrophic long-term failure mechanisms like volume swelling, embrittlement, and micro-cracking.

Traditional predictive models, such as Rate Theory, fail to forecast this long-term behavior because they require two critical accurate inputs: **Migration Barrier Energy (Em)** and **Defect Interaction Energy**.

These inputs are **impossible to measure directly** and cannot be reliably derived from classical (non-quantum) simulations.

Qualification of new structural materials takes decades and relies **on expensive, long-duration irradiation campaigns**. This dramatically slows innovation and limits deployment of advanced reactors and fusion devices.

The Solution

ASAP (Atomistic Simulation Advanced Platform)

A single, integrated platform utilizing SIESTA and Quantum Espresso (QE) to extract critical physical data.

- **Predict Stable Structures & Energies.** ASAP uses geometry optimization to find optimal structure, formation energies and interaction energies of defects.
- **Quantify Migration Barriers** (Em). The integrated Nudged Elastic Band (NEB) method automatically maps the lowest energy pathway a defect must follow, providing the quantum-accurate Em.

Characteristics computed:

- Structure and formation energy of defects
- Interaction energy of defects
- Migration barrier (Em)

Core Insight

From Quantum Data to Long-Term Reliability

- **Em Dictates Swelling**: The Migration Barrier Energy (Em) determines the relative speed of defects (vacancies and interstitials), directly controlling the rate of volume swelling.

- **Interaction Energy Determines Microstructure Fate:** ASAP quantifies the Interaction Energy between defects and damaging impurities (like Helium)

This enables **virtual screening** to predict, for example, if a material will allow defects to self-annihilate efficiently or will trap harmful Helium bubbles that cause embrittlement and micro-cracking.

Impact

Quantum Modeling to Mitigate Nuclear Swelling and Embrittlement

- **Accelerated Alloy Design**: Rapidly screens the kinetic stability of complex new alloys, allowing R&D teams to identify compositions that promote defect annihilation over clustering.

- **Reduced Qualification Time**: Cuts reliance on costly, multi-year irradiation tests by providing validated, physics-based long-term performance data.

- **Bridging the Scale Gap**: The characteristics computed with ASAP (Structure, Formation Energy, Interaction Energy, Migration Barrier) are the essential quantum-accurate outputs required for higher-level simulations (like Kinetic Monte Carlo or Phase Field Modeling) that predict long-term behavior.

Technical Validation: Publications

These publications validate the DFT methodology (SIESTA/QE codes) for simulating the formation energies, migration barriers, and interaction of radiation-induced defects (vacancies, interstitials, helium bubbles) to predict material lifetime and swelling.

ASAP automates the required SIESTA/QE calculations and analysis for rapid R&D application.

- Self-interstitials structure in the hcp metals: A further perspective from first-principles calculations
- Ab initio investigation of radiation defects in tungsten: Structure of self-interstitials and specificity of di-vacancies compared to other bcc transition metals
- Ab initio approach to the effect of Fe on the diffusion in hcp Zr II: The energy barriers
- Density functional theory calculations of helium clustering in mono-, di-, and hexa-vacancy in silicon

Technical Validation: Publications

Other examples of SIESTA use for fusion/fission applications:

- [Modeling of hydrogen retention behavior for material design for neutron multipliers:]
- [Quantum mechanical study of the influence of noble metals on the process of reduction of uranium oxides]

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