

# ***NUCLEAR ENERGY RESEARCH INITIATIVE***

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## ***Ab-Initio*-Based Modeling of Radiation Effects in Multi-Component Alloys**

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**Project Number:** 06-006

**Program Area:** Generation IV

**Collaborators:** None

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### **Project Description**

The objective of this project is to develop an original, highly accurate thermokinetic model for austenitic stainless steels based on fundamental quantum mechanical calculations. New, more accurate microstructural models are necessary for the proposed Generation IV reactor designs in order to overcome limitations inherent in the existing models. This project will take advantage of the latest developments in *ab-initio* methods and alloy theory by developing a full thermokinetic model from quantum-mechanically-derived, atomic-scale energy parameters. The model will incorporate the true temperature- and composition-dependence of the diffusion constants and provide the missing information on interstitial motion.

Atomic-scale energy parameters for austenitic Fe-Cr-Ni will be calculated with *ab-initio* methods to establish accurate diffusion constants (unlike the approximate, extrapolated values currently in use). These parameters will be calculated using kinetic and Monte Carlo simulations combined with linear response theory. The resulting model will be refined by comparing simulated radiation-induced segregation (RIS) to a comprehensive database and validated against simulated and measured void growth in austenitic alloys. In order to demonstrate the general applicability of this approach and provide further validation, the model will be extended to ferritic Fe-Cr-Ni. While the complete *ab-initio*- to microstructural-modeling approach has been developed for binary alloys, this will be the first application to a ternary system and the first time that interstitials are included.

### **Workscope**

This project will perform the following tasks in order to establish critical data and techniques for *ab-initio*-based modeling of microstructural development in complex engineering alloys:

- Perform initial *ab-initio* calculations of atomic-scale properties in pure elements and limited alloys
- Develop Fe-Cr-Ni RIS simulation and validation/refinement
- Perform more complete *ab-initio* calculations of atomic-scale properties in Fe-Cr-Ni alloy
- Develop Monte Carlo codes; Fe-Cr-Ni RIS simulation based on *ab-initio* values and Monte Carlo; further validation and refinement
- Calculate diffusion constants, void growth modeling, and Fe-Cr-Ni RIS simulation
- Perform final validation/refinement by comparison to experiments
- Extend calculations and simulations to ferritic Fe-Cr model