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Density functional calculations on structural materials for nuclear energy applications and functional materials for photovoltaic energy applications

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Abstract
Ab initio density functional theory calculations are carried out in order to predict the evolution of structural materials under aggressive working conditions such as cases with exposure to corrosion and irradiation, as well as to predict and investigate the properties of functional materials for photovoltaic energy applications. Structural metallic materials used in nuclear facilities are subjected to irradiation which induces the creation of large amounts of point defects. These defects interact with each other as well as with the different elements constituting the alloys, which leads to modifications of the microstructure and the mechanical properties. VASP (Vienna *Ab initio* Simulation Package) has been used to determine the properties of point defect clusters and also those of extended defects such as dislocations. The resulting quantities, such as interaction energies and migration energies, are used in larger scale simulation methods in order to build predictive tools. For photovoltaic energy applications, *ab initio* calculations are used in order to search for new semiconductors and possible element substitutions for existing ones in order to improve their efficiency.

