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Study of charge states of point defects and extended defects in uranium dioxide

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Recent experimental studies on oxides crystallizing in the fluorite structures (UO2, CeO2 or cubic ZrO2) have shown that under MeV electron irradiations, some atypic extended defects can be created in these materials. Faulted non-stoichiometric dislocation loops (disk-shaped interstitial oxygen layers) have already been seen. These observations raise the question about the point defect chemistry, defect clustering and charge transfers in iono-covalent insulators. Recent developments on many-body empirical potentials that use a charge equilibration method allow us to simulate various defects and their charge states.

The scope of this thesis is the study of point defects (formation and migration of point defects of different charge states) and dislocations (atomic and charge arrangements in the dislocation cores; interactions with point defects) in uranium dioxide in the framework of molecular statics and molecular dynamics.

In a second time results from these simulation will be used and integrated in a cluster dynamics algorithm to study the population and charge of clusters in uranium dioxide under irradiation.

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