Abstract Submitted
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An ab initio study of radiation damage effects on the magnetic structure of bulk Iron[1] YANG WANG, Carnegie Mellon University, G. MALCOLM STOCKS, ROGER STOLLER, DON NICHOLSON, AURELIAN RUSANU, MARKUS EISENBACH, Oak Ridge National Laboratory — A fundamental understanding of radiation damage effects in solids is of great importance in assisting the development of structural materials with improved mechanical properties for nuclear energy applications. In this presentation, we discuss our recent theoretical investigation on the magnetic structure evolution in bulk Fe after an energetic particle has disturbed the lattice by a displacement cascade. We applied a linear scaling ab initio method to the study of magnetic moment distributions in a low energy cascade for a series of time steps. The primary damage state and the evolution of the defects were simulated using molecular dynamics with a Finnis-Sinclair interatomic potential. We will show the statistics of the magnetic moments in the sample and discuss its relationship with the atomic volume distribution.

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