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**First principles finite temperature magnetism of defects in Fe using Wang-Landau method**[1] AURELIAN RUSANU, Materials Science and Technology Division, ORNL, D.M. NICHOLSON, Computational Science and Mathematics Division, ORNL, KH. ODBADRAKH, Materials Science and Technology Division, ORNL, GREGORY BROWN, Florida State University, MARKUS EISENBACH, National Center for Computational Sciences, ORNL — Magnetic structure of materials with defects presents a strong dependence on local atomic arrangements. This dependence affects mechanical, magneto-caloric, and magnetization properties. Insights into thermodynamic and magnetic fluctuations at defects in Fe are obtained from first principle analysis by deploying the first principle local self consistent multiple scattering method(LSMS) and Wang-Landau statistical method. The computation of thermodynamic properties requires the sampling of a large number of configurations. To reduce the computational effort a Heisenberg model will be used to speed the configuration sampling procedures. The approach will be demonstrated for Fe systems and will address the magnetic structure of defects.

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