**Large Scale Ab Initio Calculations for Magnetic Materials and Alloys**  
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**Abstract**

The ability to understand and control the properties of materials is of paramount importance in a wide range of applications ranging from structural materials at the largest scale to functional materials for nanotechnology applications. While current computational capabilities are able to provide highly accurate first principles results for simple, idealized systems or to use approximate models for larger systems, providing capabilities for the ab initio investigation of realistic materials including defects and disorder at operating temperatures will require substantial increases in available computational resources.  This poses distinct challenges that go beyond today’s computational capabilities. We are working towards providing these capabilities by expanding the boundaries of the capabilities of our computational tools, Locally Self-consistent Multiple Scattering Theory (LSMS) and Wang-Landau Monte-Carlo simulations, to achieve:

•First principles based statistical physics of alloys and magnetic materials

•Magnetic properties of real materials

•Fully relativistic full-potential DFT calculations for heavy elements and magnetic systems