Modeling disorder in crystalline materials using systematically improvable correlated methods (Correlated_Disorder)

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This proposal aims to advance the modeling of disordered correlated-electron materials by developing novel ab-initio quantum chemistry methods that challenge the prevailing dominance of density functional theory (DFT) in this area. By harnessing recent breakthroughs in Green's function techniques, machine learning, and advanced mathematical models, we propose a comprehensive suite of tools for predicting spectral and thermodynamic properties of disordered materials.

The methods developed in this proposal, based on finite temperature Green's function approaches, will enable accurate and costeffective simulations of disordered systems, overcoming the limitations of current approaches which rely predominantly on DFT. The proposed techniques will facilitate the study of a wide range of materials where disorder is a key factor, such as high entropy alloys, superconductors, and catalytic surfaces. Additionally, we will develop machine learning models trained on ab-initio Green's function data and integrate them with ab-initio molecular dynamics to study dynamic processes in disordered systems. Finally, we will also deliver tools for learning material specific DFT functionals from the ab-initio Green's function data providing an insight into the functional design.

This project aims to open new frontiers in quantum chemistry and materials science, fostering interdisciplinary collaborations and providing a foundation for the next generation of computational tools. The anticipated outcomes include enhanced predictive capabilities for disordered systems and improved insights into the design of DFT functionals, contributing significantly to the fundamental scientific understanding of correlated materials.