



Collaborative Research: Element: Development of MuST, a Multiple Scattering Theory based Computational Software for First Principles Approach to Disordered Materials

Award #: NSF-OAC -1931525,
1931367,1931445

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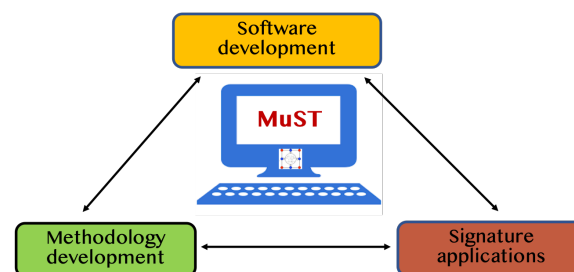
Motivation:

Disorder is a common feature of real materials which can dramatically affect their properties. Proper ab-initio study of disorder effects is critical for understanding and harnessing the role of disorder in material design and functionalities.

<https://github.com/mstsuite/MuST>

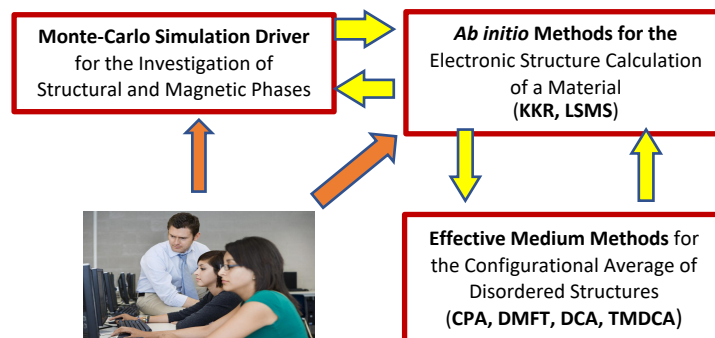
Our Goals:

- **Software development:** open-source ab-initio numerical framework for systems with disorder.
- **Method development:** expand the existing capabilities of ab initio codes to study strong disorder.
- **Signature applications:** explore disorder effects in disordered metals, high entropy alloys, semiconductors, and topological insulators.



Software Framework of MuST

A computational tool for the study of quantum phenomena in disordered materials



Intellectual Merit:

- Develop an ab-initio numerical framework for systems with weak and strong disorder.
- Create a truly scalable ab-initio multiple-scattering theory approach that utilizes petascale and future HPS resources.
- Enable exploration and deeper understanding of disorder-driven quantum phenomena in materials.

Broader Impacts:

- Provide research community with the open-source ab-initio codes for disordered systems.
- Undergraduate and graduate student training.
- User training via workshops and public online educational materials.
- Outreach programs for K-12 students to encourage minorities and underrepresented groups in STEM fields.