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

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MuST: an open-source software for ab-initio study of disordered quantum materials

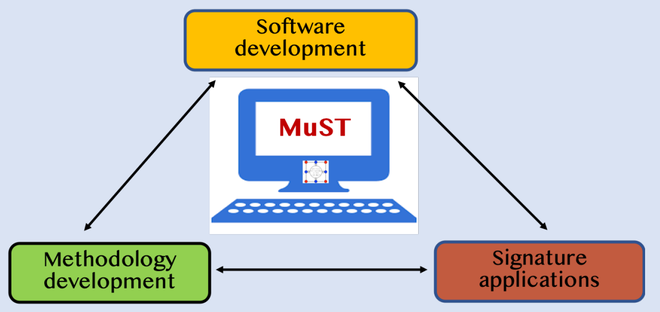
Motivation

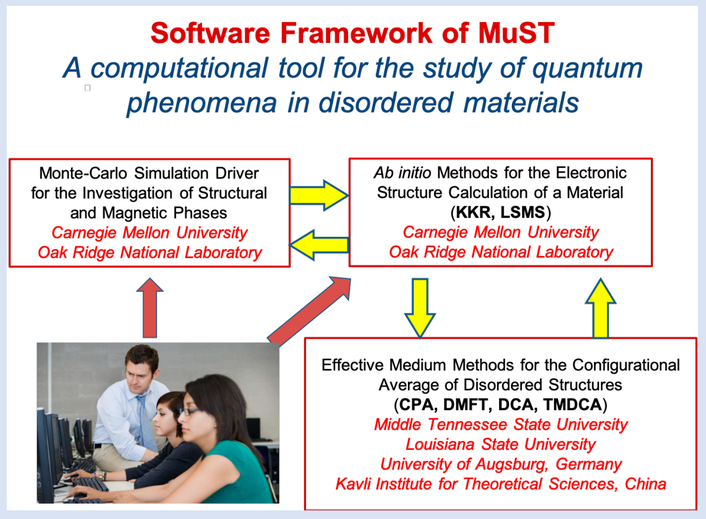
Disorder (impurities, defects) is a common and often unavoidable feature of real materials. It can have profound effects on electronic, magnetic, structural, and transport properties of materials.

Understanding and harnessing the role of disorder is critical for controlling and utilizing the functional properties of quantum systems with disorder. A careful theoretical and numerical analysis to be done is required.

Our Goals

- **Provide an open-source** ab-initio numerical framework for systems with disorder.
- **Create a truly scalable multiple-scattering theory** approach for the first principle study of quantum materials.
- **From models to real materials**: expand the existing capabilities of ab initio codes to study strong disorder effects i.e., disorder-driven quantum phase transitions, transport and electron localization (currently available at model Hamiltonian level only).
- **Method development to enable exploration of disorder effects in a variety of materials**: disordered metals, high entropy alloys, semiconductors, and topological insulators.
- **Enable researcher to perform ab-initio calculations for disordered systems** that are presently out of reach to most researchers.





https://github.com/mstsuite/MuST

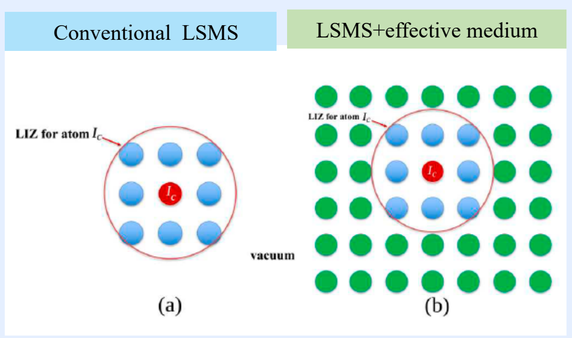
The MuST package codes: KKR, KKR-CPA, LSMS, DCA TM-DCA

Recent MuST Development and Application

Method development: combining super cell+effective medium methods.

Strong disorder leads to spatial localization of waves such as electrons and phonons and is expected to play a central role in energy materials.

The existing capabilities of the state-of-the-art DFT codes in MuST code are limited to metallic or metallic alloy systems only. A combination of LSMS with effective medium methods is needed to study strong disorder electron localization.



To test such ideas, we have constructed TMDCA+LSMS a new embedding scheme and applied it to 3D Anderson model.

This approach opens the path towards the development of the typical medium embedding scheme for O(N) multiple scattering DFT methods. [1] PRB 100, 054205 (2019).

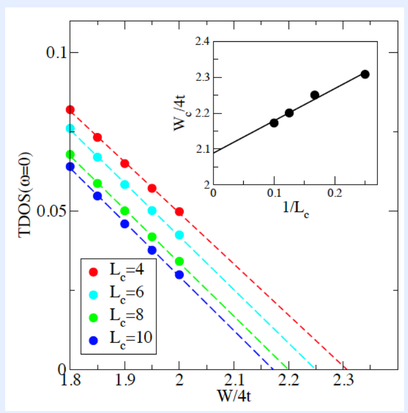


Fig: Anderson localization is identified by vanishing TSOS(w=0). Inset: extrapolation of the critical disorder strength Wc of the transition to the thermodynamic limit.

From models to real materials: ab-initio study of electron localization in substitutional alloy systems

To study electron localization in real materials, recently, our effective medium typical medium theory has bee implemented within the DFT by employing the EMTO-basis set. [2] PRB 101, 014210 (2020).

The developed typical-medium ab-initio scheme was applied to study the evolution of the the impurity band appearing in the hypothetical Li_cBe_{1-c} alloy, a simple cubic system with one-atom per unit cell.

Signatures of Anderson localization, band narrowing, and split-off impurity bands have been observed.

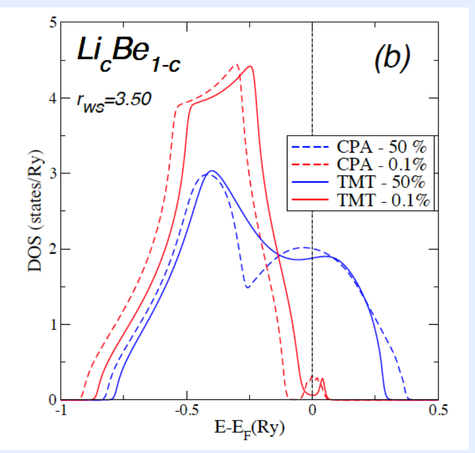
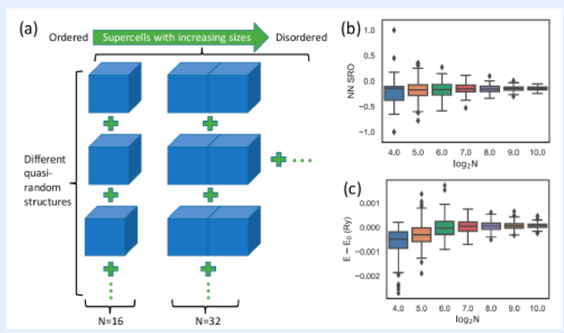


Fig: Average DOS and Typical DOS computed using CPA and TMT effective medium.

Using LSMS Code from MuST for Machine Learning

Disordered supercell DFT methods are very much limited by the system size ($O(N^3)$ scaling). The MuST LSMS code is a powerful super-cell code with linear scaling which allows treating large systems beyond 10,000 atoms.

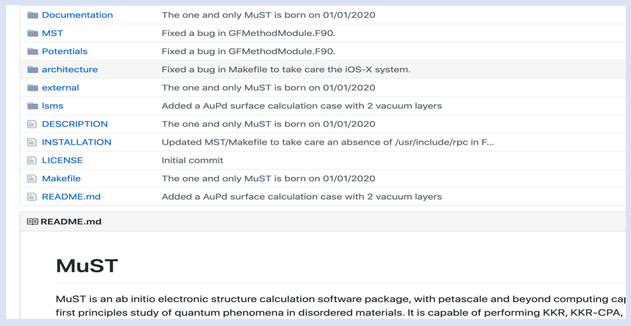
Recently, LSMS code has been used to generate ab-initio data for machine learning study of the high-entropy alloys. [3] arXiv: 1906.02889.

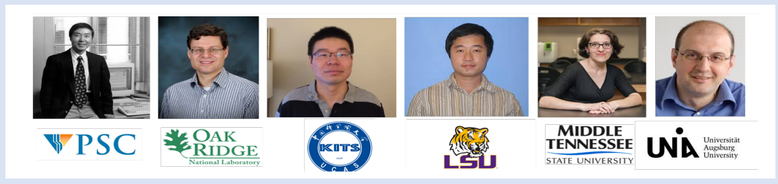


Broader Impacts

Community Building

- January 2020: Open-source MuST software is now available at https://github.com/mstsuite/MuST
- Wiki page on GitHub: user manuals, tutorials and application examples
- Integrating MuST as a community code on NSF/XSEDE (in future)





Core Team: Yang Wang, Markus Eisenbach, Yi Zhang Ka Ming Tam, Hanna Terletska, Liviu Chioncel

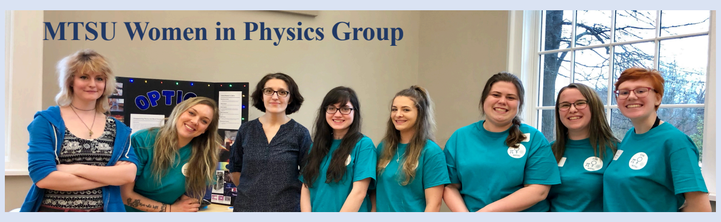
Workforce Development

- Summer interns at CMU (XSEDE EMPOWER program).
- Physics undergraduate students B. Sc. Theses.

Aric Moilanen

Jaron Hengstenberg

- Graduate student training at LSU.
- Workshops on computational study of quantum materials.



Educational Outreach

- Annual LSU Beowulf Boot Camp for Louisiana high School and middle school students & Louisiana Teachers.

- Annual Quantum Day Physics Workshop at Pittsburg Quantum Institute.
- Annual Expanding Your Horizon Conference for middle and high-school female students at MTSU.