LA-SiGMA

Louisiana Alliance for Simulation-Guided Materials Applications

Spring Seminar Series
3:30pm - 4:30pm, Wednesday, January 23, 2013
Tilton Hall 305, Tulane University

High-Throughput Searches for Electronic Materials in AflowLib.org: Robustness and Fragility of Topological Insulators

by

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Accelerating discovery and design of new electronic materials through computational screening involves filtering of a large number of candidates according to a set of desired properties [1]. Current efforts have relied mostly on costly and time-consuming trial and error procedures. In this talk we will show that by defining a reliable and accessible descriptor χ_{TI}, which represents the topological robustness or feasibility of the candidate, and by searching the quantum materials repository *aflowlib.org*, we have automatically discovered 28 new topological insulator materials (TI) (some of them already known) in five different symmetry families [2].

Topological insulators (TI) are becoming one of the most studied classes of novel materials because of their great potential for applications ranging from spintronics to quantum computers. To fully integrate TI materials in electronic devices, high-quality epitaxial single crystalline phases with sufficiently large bulk band-gaps are necessary. The novel family discovered by our computational procedure includes peculiar ternary compounds, which could have been hardly anticipated without high-throughput means. The presented search model, by relying on the significance of repositories in materials development, opens new avenues for the discovery of more TIs in different and unexplored classes of systems [2].

If time allows, we will introduce and discuss a novel library of thermal conductivity properties for a nano-sintered half-Heuslers semiconducting powders [3].

[1] Curtarolo, G. L. W. Hart, M. Buongiorno Nardelli, N. Mingo, S. Sanvito, and O. Levy, "*The high-throughput highway to computational materials design*", Nature Materials (2013).
[2] K. Yang, W. Setyawan, S. Wang, M. Buongiorno Nardelli, and S. Curtarolo, "*A search model for topological insulators with high-throughput robustness descriptors*", Nature Materials **11**(7), 614-619 (2012).
[3] Montaña, Wang, Mingo, Curtarolo, "*High-throughput thermal transport characterization of 500,000+ Heuslers nano-powders*", (2013).

About the speaker

After studying Electrical Engineering and Physics in Padova, Italy, Stefano Curtarolo (SC) received his PhD in Materials Science from MIT in 2003. Since then, he was faculty of Materials Science and Physics at Duke University. During his time at Duke, SC received the ONR-Young-Investigator, the NSF-Career, and the Presidential PECASE Awards in addition to the International Union of Pure and Applied Physics - Young Scientist Prize in Computational Physics. SC was promoted to Associate in Oct.2008, to Full Professor in Feb. 2012 and he started the Center for Materials Genomics in July 2012. Currently he has more than 80 refereed publications and more than 120 invited departmental seminars and talks in national and international conferences. At Duke University, the SC's group released the "on-line ab-initio binary phase diagram database" containing free energy information for more than 1,500 binary intermetallic alloys (http://materials.duke.edu/apool.html) and the "high-throughput electronic structure consortium repository" containing more than 450,000 fully ab-initio electronic characterization for inorganic compounds (http://www.aflowlib.org). [http://materials.duke.edu/auro/cv.pdf].