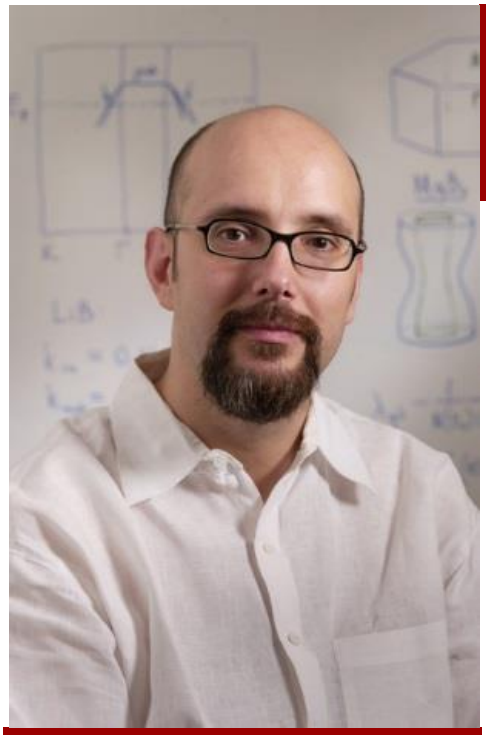

Spectral Sampling in Accelerated Materials Discovery

Date : **Tuesday, September 2, 2014**

Time : **6:00 pm – 7:00pm**

Location : **Guyon Auditorium**

Professor Stefano Curtarolo

Departments of Physics, and Mechanical Engineering and Materials Science

Duke University, Durham, NC

Abstract: In this presentation, we show how to use on-line resources to accelerate materials development. The test bed will be thermoelectric systems and topological insulators. We will also discuss how to encode electronic structures into materials fingerprints, so that libraries of calculations can be mined for finding novel unknown superconductor correlations. Some discussion will be given about a quick API interface. Research is sponsored by DOD, DOE, NIST, DHS, and Cray Computers.

After studying Electrical Engineering and Physics in Padova, Italy, Stefano Curtarolo received his PhD in Materials Science from MIT in 2003. Since then, he was a faculty of Materials Science and Physics at Duke University. During his time at Duke, Stefano Curtarolo received the ONR-Young-Investigator, NSF-Career, and Presidential PECASE Awards; the International Union of Pure and Applied Physics - Young Scientist Prize in Computational Physics; the Stansell Research Award; and the 2013 MURI Award for strategies in element replacement. Currently he has ~95 refereed journal publications and >140 invited departmental seminars and presentations in national and international conferences. At Duke University, the Stefano Curtarolo's group started the ``on-line ab-initio aflowlib.org'' consortium containing free energy information and electronic characterization of more than 600,000 entries/compounds.