Carnegie Mellon University Materials Science & Engineering

presents

Don't Cry Over Spilled Entropy

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ABSTRACT:

Critical understanding of large amount of data exposes the unavoidability of disorder and leads to new descriptors for discovering entropic materials. The formalism, based on the energy distribution spectrum of randomized calculations, captures the accessibility of equally-sampled states near the ground state and quantifies configurational disorder capable of stabilizing high-entropy homogeneous phases. The methodology - applied to disordered refractory 5-metal carbides (promising candidates for high-hardness, high-melting point applications) – uncovers scientific surprises. Directions for entropic reciprocal ceramics and spectral convolution methods are also discussed. Research sponsored by DOD-ONR.

BIOGRAPHY:

Dr. Curtarolo research interests lie at the intersection of materials science, artificial intelligence and autonomous discovery of new materials. After studying Electrical Engineering and Physics in Padova, Italy, SC received his MS in Physics from Penn State University in 1999, and a PhD in Materials Science from MIT in 2003. Since then, he has been on the faculty of Materials Science at Duke University. During his time at Duke, SC received the DOD-ONR-Young-Investigator (2007), the NSF-Career (2007), the Presidential PECASE Awards (2008), the International Union of Pure & Applied Physics -Young Scientist Prize in Computational Physics (2011), the Stansell Research Award (2013), Fellowship by APS (2013) and the 2013 MURI Award for strategies in rarematerials replacement. SC was promoted to Associate and Full Professor in 2008, and 2012, respectively. In 2015 SC received the "Friedrich Wilhelm Bessel Research Award" from the Alexander von Humboldt Foundation. SC has 160+ refereed publications, 220+ invited departmental seminars and talks in national and international conferences, and 10000+ scientific citations. At Duke University, the SC's group started and maintains the quantum-cloud aflow.org consortium containing materials information and tools for more than 4.000,000+ compounds. His teams focus on developing autonomous daemons for materials discovery as well as tackle problems of synthesizability and manufacturability of amorphous/disordered systems.

> Doherty Hall 2210, 11:30AM Friday, October 4, 2019