Department of Materials Science and Engineering

Iby and Aladar Fleischman Faculty of Engineering
Tel Aviv University

הפקולטה להנדסה ע"ש איבי ואלדר פליישמן
אוניברסיטת תל אביב

המחלקה למדע והנדסה של חומרים

*You are cordially invited to attend this seminar to be held on*

***Sunday, February 4th, 15:00***

***Room 206, Wolfson Mechanical Engineering Building***

# Novel high-entropy carbides discovered by synthesizability descriptors


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High-entropy materials have attracted considerable interest due to their combination of potentially unique properties and promising technological applications. Predicting their formation from previously known parameters remains the major hindrance to the discovery of new systems. In this seminar, we introduce a descriptor - entropy forming ability - for predicting the synthesizability of such systems from first principles calculations. 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 potentially leading to high-entropy homogeneous single-phases. The methodology is used to seek for disordered refractory 5-metal carbides | potential systems for ultra-high temperature applications. The descriptor correctly predicts a set of candidates that are experimentally synthesized as novel high-entropy homogeneous phases, validating the ansatz of the model. The method has the potential to accelerate the search and development of high-entropy crystalline systems by rationally combining first principles approaches with experimental synthesis.


***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 (Physics, Chemistry and Electrical Engineering included). 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 rare-materials 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, and currently he is spending his sabbatical time at the Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin. As of October 2017, SC has more than 130+ refereed publications, 200+ invited departmental seminars and talks in national and international conferences, and 6000+ 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.

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