

THE MATERIALS SCIENCE AND ENGINEERING DEPARTMENT FALL COLLOQUIUM SERIES PRESENTS:

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Accelerating thermoelectric materials discovery - Uniting experiment and computation

Over the last decade, significant effort has been devoted to creating computational predictive frameworks for predicting the thermoelectric performance of materials. Such efforts shine light into reciprocal space, where we often have less chemical intuition, and thus enable the accelerated down-selection of candidate materials. Computational predictions, interrogated by experiment, has revealed new classes of thermoelectric materials, thereby validating this approach as a key tool in the search for thermoelectric materials. However, we now face a new problem: We have more predicted candidates than experimental bandwidth to test these candidates. Further, the expansion of thermoelectric training sets for machine learning remains quite slow. As such, our current efforts are focused on developing the infrastructure to accelerate synthesis and characterization of thermoelectric materials by x50 without significant sacrifices in material or data quality. These efforts are inspired by develops over the last three decades in combinatorial thin film growth, but are focused instead on bulk materials. Efforts to develop high throughput weighing, milling, consolidation, and transport measurements will be discussed in the context of pnictide and chalcogenide thermoelectric materials.

Eric Toberer is an Associate Professor in the Physics Department at the Colorado School of Mines, Director of the Materials Science Program with a co-appointment at the National Renewable Energy Laboratory. Prior to arriving in Colorado, he was a post-doc at the California Institute of Technology where he worked with Jeff Snyder on thermoelectric materials. As a result of these efforts, Dr. Toberer received the 2011 International Thermoelectric Society Young Investigator Award. In 2015, he received the Cottrell Scholar Award for simultaneous excellence in teaching and scholarship and the NSF CAREER award and the PECASE in 2019. Dr. Toberer conducted his graduate work with Ram Seshadri at the University of California, Santa Barbara (2002–2006) on the synthesis of hierarchically porous materials within the Materials Department and received his undergraduate degree in Chemistry from Harvey Mudd College.

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