First-Principles Optimization and Discovery of Materials for Energy Conversion and Storage

Materials innovations require considerable time and resources. This presentation will discuss the use of first-principles modeling for optimizing the properties of materials over relevant time and length scales and for narrowing down the choice of candidate materials for target applications. The focus will be on minimizing heat transport in thermoelectric semiconductors and on producing hydrogen fuels photocatalytically by cleaving water molecules under solar illumination. An overview of the state of the art in electronic-structure calculations will be given and progress in overcoming the size and accuracy limits of these techniques will be highlighted.

BIOGRAPHY

Dr. Ismaila Dabo is an Associate Professor in the Department of Materials Science and Engineering at Penn State University with joint appointments in the Penn State Institutes of Energy and the Environment, and in the Penn State Materials Research Institute. He received a Ph.D. in Materials Science and Engineering from MIT. His recent awards include the Corning Chair in Materials Science and Engineering (2020), Montgomery-Mitchell Teaching Award (2019), and NSF Career Award (2017). His research is strongly driven by collaboration with experimentalists with the ultimate goal of breaking down the complexity of materials design problems.