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Exploring Materials Properties via Simulations and Experiments for Thermoelectricity[1] ARTEM KHABIBULLIN, LILIA WOODS, GEORGE NOLAS, University of South Florida — Thermoelectricity is an alternative route for energy conversion and suitable materials play an important role for enhanced efficiency of related applications. The optimization of the thermoelectric transport relies on the microscopic understanding of the materials internal properties, such as electronic structure characteristics. Simulations methods and effective medium theories are utilized to investigate advantageous features in materials composed of earth-abundant elements. Some general trends in the electronic structure influencing the transport are formulated for chalchogenide and clathrate systems suitable for thermoelectricity. We emphasize the importance of theoretical and computational efforts not only to identify existing classes, but also predict new structures with desirable internal characteristics for effective materials design and optimization.

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