## "固体所青联会"第二十期学术论坛

报告题目: Predicting the thermoelectric properties of several bulk and low-dimensional systems

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举办单位: 中科院固体物理研究所青年联合会

中科院青年创新促进会合肥物质科学研究院小组

报告内容: Thermoelectric materials can directly convert heat into electricity and vice versa. Such materials utilize the Seebeck effect for power generation and the Peltier effect for refrigeration. As the global energy crisis and environment pollution becoming more and more serious, the search for new thermoelectric materials is of important significance. In this talk, the thermoelectric properties of several bulk and low-dimensional systems are investigated by using a multiscale approach which includes first-principles method, Boltzmann theory, molecular dynamics simulations, and etc. Our theoretical works predict very high ZT values for some example systems such as bismuth, black phosphorous, and transition-metal dichalcogenide, which deserve further experimental investigations and confirmations.