

APCTP SEMINAR

Influence of Strain on the High Temperature Thermoelectric Behavior of Scandium nitride - A Combined First- principles and Boltzmann Transport Formalism approach

Date/Time 17:00-18:00, May 11 (Tue.), 2021

Venue APCTP 512 Seminar Room

Speaker Iyyappa Rajan Paneer Selvam (APCTP)

Abstract While most of the thermoelectric materials work well only at low and mid temperatures, high temperature thermoelectric materials are equally important for future energy conversion applications. The applications include but not limited to the operation of deep spacecraft missions and the conversion of the waste heat from the nuclear reactors and high-temperature industrial reactors into electrical power generation. To accomplish this demand, I will talk about a few insights of the application of strain in scandium nitride (ScN) towards high temperature thermoelectric performance. This presentation is based on the results obtained from the first-principles density functional theory (DFT) calculations and Boltzmann transport formalism along with an experimental literature validation wherever possible. In this talk, I will also elaborately discuss the transport properties such as Seebeck coefficient, electrical and thermal conductivities which are calculated using the various physical parameters of materials to obtain the optimum thermoelectric power-factor and figure-of-merit.

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