



Warwick Centre for Predictive Modelling Seminar Series

**Electronic, thermal, and thermoelectric
transport in nanostructures**

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LIB1, Lower Level, Main Library

Abstract: Recent advancements in nanofabrication have enabled the realization of devices and materials with feature sizes that vary from 100s down to a few nanometres. In these structures, the length scale can be used as a degree of freedom to explore material properties 'by design'. Several technologies benefit from such advancements, i.e. advanced transistors, photovoltaics, solid-state-lighting, thermoelectrics, etc. In all these cases, an understanding of transport and atomistic phenomena is essential in addressing material properties.

In this talk I present our recent work on electronic and thermal transport in nanostructures. A variety of techniques is employed such as atomistic tight-binding, valence-force-fields, semiclassical transport and quantum transport. I then explain how efficient thermoelectric materials can be realized. More specifically, I explain how bandstructure effects can be used to improve the thermoelectric power factor of low-dimensional systems, how nanoscale disorder can reduce thermal conductivity, and how combining the two effects, enhanced thermoelectric ZT figure of merit can be achieved. Design engineering techniques for a series of nanoscale materials such as nanowires, quantum wells, graphene ribbons, and nanocomposites are presented.

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