



School of Nano Science



IPM Condensed Matter &  
Statistical Physics Group

## Weekly Seminar

### Thermal transport engineering in nano-structured materials using classical molecular dynamics simulation

Invited Speaker:

**Dr. Ali Rajabpour<sup>1,2</sup>**

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#### **Abstract:**

Today, thermal transport management in nanoelectronic devices is an important factor in their design, efficiency and lifetime. Moreover, thermal conductivity plays an important role in figure of merit of thermoelectric devices. Because of its fundamental aspects and important technological applications, nanoscale heat transport has emerged as an interdisciplinary area of research involving condensed matter physics, material sciences, electrical and mechanical engineering, etc. Heat transfer at nanoscale is essentially different from that at macroscale and is governed by the mean free paths of heat carriers in materials. In this presentation, I will talk about the unusual thermal behavior of materials at nanoscale. Using classical molecular dynamics simulation approach some results about engineering thermal transport in graphene-based nanostructures by applying strain, nitrogen doping, hydrogen functionalization and etc. will be presented. Boundary effect, interface effect (Kapitza thermal resistance) on thermal transport of nanostructures will also be discussed.

Wednesday, 23<sup>th</sup> of Farvardin (1396) (April 12<sup>th</sup>, 2017), 14:00-15:00  
Farmaniyeh seminar room