School of Nano Science (IPM)

School of PHYSICS

Condensed Matter & Statistical Physics Group (IPM)

Weekly Webinar

Ab initio prediction of magnetic properties

Speaker: **Dr. Mojtaba Alaei**

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One of the progressing material science field is to design new materials using computer simulations. In this regard, the most important issue is correct prediction of material properties. One of the popular method for prediction of material properties is ab initio methods such as density functional theory (DFT). But because of technical difficulties, it is hard to derive temperature dependent properties of magnetic materials, such as transition temperature, from such methods directly. Therefore, we combine DFT and methods such as Monte-Carlo (MC) (DFT+MC) to predict magnetic material properties versus temperature. In this lecture, we want to discuss about calculation of magnetic properties using DFT+MC. On this subject, we mention several works which done in QSM group including writing and developing ESpinS package.

Wednesday, 12 August 2020 (۲۲ مرداد ۱۳۹۹), 14:00-15:00

Virtual Meeting Room (please log in as a guest):
https://www.skyroom.online/ch/schoolofphysics/school-of-nano-science