



School of Nano Science



IPM Condensed Matter &
Statistical Physics Group

Weekly Seminar

Investigation of the electrical properties of Borophene, and Borophene Nanoribbons by density functional theory

Invited speaker: *Dr. Sahar Izadi*

School of Nano Science, IPM

Abstract:

After the discovery of graphene, other two dimensional (2D) materials were theoretically predicted and experimentally synthesized, such as silicene, germanene, stanene, and black phosphorene. Recently, a new member has been added to the single element 2D family that unlike the others, doesn't have a unique structure. Borophene, a single layer of boron atoms, has recently been synthesized by two independent groups [1,2]. It is interesting that the results of these experiments are different and show two-dimensional boron polymorphs. Accurate analysis of scanning tunneling microscopy and density functional theory (DFT)-based simulations showed that three different phases of the borophene, i.e. $2Pmmn$, χ_3 and β_{12} , had been synthesized in the two mentioned experiments. Experimental and theoretical investigations showed that all the synthesized borophene sheets were metal. A lot of research has been devoted to studying the outstanding properties of borophene sheets in the last years. In this talk, I introduce different types of freestanding 2D-boron sheets, including corrugated borophene and completely planar borophene sheets. The electrical properties of these structures and their nanoribbons are investigated by DFT. A spin anisotropy is predicted at the edges of specific borophene nanoribbons that makes them completely different from graphene nanoribbons. The spin anisotropy can be considered as a new degree of freedom in spintronic applications.

Wednesday, 24 Bahman 1397 (Feb 13, 2019), 14:00-15:00

Seminar Room (classroom A), Farmanieh Building, IPM