



School of Nano Science



IPM Condensed Matter &
Statistical Physics Group

Weekly Seminar

Optical absorption properties of few-layer phosphorene

Invited speaker:

Dr. Zahra Torbatian

School of Nano Science, IPM

Abstract:

We investigate the optical absorption and transmission of few-layer phosphorene in the framework of ab initio density functional simulations and many-body perturbation theory at the level of random phase approximation. In bilayer phosphorene, the optical transition of the valence band to the conduction band appears along the armchair direction at about 0.72 eV, while it is absent along the zigzag direction. This phenomenon is consistent with experimental observations. The angle-resolved optical absorption in few-layer phosphorene shows that it is transparent when illuminated by near grazing incidence of light. Also, there is a general trend of an increase in the absorption by increasing the number of layers. Our results show that the bilayer phosphorene exhibits greater absorbance compared to that of bilayer graphene in the ultraviolet region. Moreover, the maximal peak in the calculated absorption of bilayer MoS₂ is in the visible region, while bilayer graphene and phosphorene are transparent. Besides, the collective electronic excitations of few-layer phosphorene are explored. An optical mode (in-phase mode) that follows a low-energy \sqrt{q} dependence for all structures, and another which is a damped acoustic mode (out-of-phase mode) with linear dispersion for multilayer phosphorene are obtained. The anisotropy of the band structure of few-layer phosphorene along the armchair and zigzag directions is manifested in the collective plasmon excitations.

Wednesday, 3 Mehr 1398 (September 25, 2019), 14:00-15:00

Seminar Room (Classroom A), Farmanieh Building, IPM