



School of Nano Science



IPM Condensed Matter &
Statistical Physics Group

Weekly Seminar

Understanding Metal Cluster with Theoretical Spectroscopy

Invited Speaker:

Dr. Zahra Jamshidi

Chemistry and Chemical Engineering Research Center of Iran

Abstract:

Atomic and molecular clusters exhibit unique chemical and physical properties that are markedly different from the bulk phase. For small metal clusters, chemical reactivity as well as optical and magnetic properties are known to depend strongly on the cluster size, but it is still very difficult to predict structural and electronic properties from knowledge of cluster composition and size only. To improve our understanding of these important model systems, the experimental and theoretical techniques are combined. Therefore, the development of theoretical spectroscopy is essential to predict the UV-Vis and IR spectra near the experimental results. However, such calculations face multiple challenges. The emergence of metallic behaviour manifests itself in the closing of the HOMO-LUMO gap and the appearance of multiple possible spin states. Furthermore, for heavy metal considering the relativistic effect and spin-orbit coupling are crucial. Accurate theoretical prediction of metal clusters spectra despite of these challenges is the interest of our research.

Wednesday, 3 Aban 1396 (October . 25, 2017), 14:00-15:00

Seminar Room (classroom A), Farmanieh Building, IPM