



School of Nano Science

IPM Condensed Matter and
Statistical Physics Group

Weekly Seminar

Development of Ab Initio Quantum Chemistry Techniques for Multi-component Systems with Applications in Quantum Theory of Atoms in Molecules

Speaker:

Dr. Mohammad Goli

School of Nano Science, IPM

Abstract:

The extended theory of multi-component quantum theory of atoms in molecules (MC-QTAIM) is able to extract atoms in molecules (AIM) and quantify their properties for systems considered beyond the clamped-nuclei approximation. In order to study these types of systems, a variety of non-Born-Oppenheimer methods have been developed. In these methods, all electrons and specified nuclei are treated quantum mechanically on equal footing using orbital-based techniques. This type of ab initio, non-Born-Oppenheimer electronic structure approach aims to solve the time-independent Schrodinger equation for a multi-component system.

Wednesday, 25 Farvardin 95 (13 April, 2016), 2-3 pm

Farmaniyeh seminar room