



School of Nano Science



IPM Condensed Matter &  
Statistical Physics Group

## Weekly Seminar

### **A quantitative model for oxygen uptake and release in a family of hemeproteins**

Invited Speaker:

***Leonardo Boechi***

*Instituto de Calculo, University of Buenos Aires, Argentina*

#### ***Abstract:***

In this talk, we will present a physical–chemical model, which uses data obtained exclusively from computer simulations, to describe the uptake and release of oxygen in a family of hemeproteins. Through a rigorous statistical analysis we demonstrate that our model successfully recaptures all the reported experimental oxygen association and dissociation kinetic rate constants, thus allowing us to establish the key factors that determine the rates at which these hemeproteins uptake and release oxygen.

**Wednesday, 25 Mordad 1396 (Aug. 16, 2017), 14:00-15:00**

**Seminar Room (Classroom A), Farmanieh Building, IPM**

**Organized by the School of Nano Science**