



قطب علمی
سیستم‌های پیچیده
و ماده چگال



سمینار هفتگی ماده چگال نرم

**A short report of the research activity during my visit from
Abdus Salam International Centre for Theoretical Physics**

ارائه دهنده

ندا رفیعی

پژوهشگاه دانش‌های بنیادی

The main purpose of my visit from Abdus Salam International Centre for Theoretical Physics (ICTP) was to improve my knowledge and experience in my field of research which is molecular dynamics simulation of biomolecules; in this respect, I attended some selected courses in ICTP and SISSA (Scuola Internazionale Superiore di Studi Avanzati) among which were *molecular dynamics* and *advanced sampling techniques*. I learned the most important techniques for doing a simulation and analyzing the results in a correct and meaningful manner. Besides, I started a new project in collaboration with Prof. Ali Hassanali in Condensed Matter and Statistical Physics (CMSP) group. The aim of this project is using classical molecular dynamics simulation to understand the mechanism by which amyloid beta (AB) protein interacts with silica surface and how AB fibrillation is affected by the surface. It is well known that fibrillation of AB leads to plaque formation and neural cell death which occurs in neurodegenerative diseases such as Alzheimer's disease. Recent studies suggest that some surfaces, such as gold, inhibit the aggregation process, while some others like silica can accelerate it depending on many factors including surface structure and morphology, surface chemistry, surface charge density, temperature and pH of the environment in which the interaction of protein with surface is studied, concentration of protein in solution, etc.

In this lecture, I will summarize the aim of this project, the methodology that we use and the results that we obtained up to now. I will also give an outlook for the rest of this project.

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