



School of Nano Science



IPM Condensed Matter &
Statistical Physics Group

Weekly Seminar

Multi scale modeling of microtubule under influence of external electric field: molecular dynamics and coarse grain methods

Invited Speaker:

Dr. A. Lohrasebi

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Abstract:

Microtubule (MT) rigidity and response to 2450 MHz electric field were investigated, via multi scale modeling approach. For this purpose, six systems were designed and simulated to consider all types of feasible interactions between α and β monomers in MT, by using all atom molecular dynamics method. Subsequently, coarse grain modeling was used to design different lengths of MT. Investigation of effects of external 2450 MHz electric field on MT showed MT less rigidity in the presence of such field, which may perturb its functions. Moreover, an additional computational setup was designed to study effects of 2450 MHz field on MT response to AFM tip. It was found, more tip velocity led to MT faster transformation and less time was required to change MT elastic response to plastic one, applying constant radius. Moreover it was observed smaller tip caused to increase required time to change MT elastic response to plastic one, considering constant velocity. Furthermore, exposing MT to 2450 MHz field led to no significant changes in MT response to AFM tip, but quick change in MT elastic response to plastic one.

Wednesday, 28 Tir 1396 (July. 19, 2017), 14:00-15:00

Seminar Room (classroom A), Farmanieh Building, IPM

Organized by the School of Nano Science