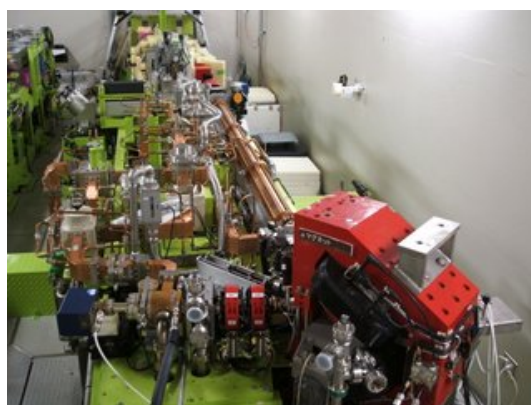


FEL-TUS Chemical Physics Seminar



日時：令和元年 10 月 22 日(火) 13:30 ~ 14:30

場所：東京理科大学神楽坂キャンパス 10 号館 1012 ゼミ室

講師：Dr. Phuong H. Nguyen

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題目：Development and application of equilibrium and non-equilibrium simulation methods to study the assembly and disassembly of biomolecules

概要：

Many peptides and proteins self-associate to form oligomeric and high-order structures. Among them, amyloid proteins can be the cause of various neurodegenerative diseases such as Alzheimer's, Parkinson's diseases, or can be functional and involve for example in protein storage, silk formation, melanin production, immune response and biofilm formation. In order to utilise the robustness of amyloids for positive function, the process of amyloid assembly and disassembly must be tightly regulated. In the first part of this talk, I will present our recent results on the assembly and disassembly processes of various peptides. The assembly process is simulated by equilibrium molecular dynamics or Monte Carlo simulations using all-atom or coarse-grained protein lattice models, while the disassembly process is induced either by infrared laser or ultrasound and followed by nonequilibrium molecular dynamics simulations. In the second part, I will present two recently developed methods including the ultrasound induced bubble cavitation and focused ultrasound molecular dynamics simulations. The applications of these methods are demonstrated on various problems such as bubble cavitation induced amyloid clearance, cell membrane formation, nanomotor propulsion and lipid membrane disruption. The implication of results on the drug delivery is discussed in some details.

事前登録は必要ありません。関連分野の学生・研究者の来聴を歓迎いたします。

世話人 化学科 築山光一（内線 5729）・FEL センター 川崎平康（野田 6200）