JGP Seminar

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"Molecular Multibody Dynamics"

Abstract

Bond length, bond angle, and torsion angle internal coordinates are more natural than Cartesian absolute coordinates for describing the conformation of molecules such as proteins. However, it is not trivial to formulate and solve the classical equations of motion in internal coordinates. In this lecture we will show how the apparent complexity of multibody dynamics, its "sea of algebra", can be conquered in surprisingly elegant ways by 6-dimensional spatial vectors, spatial operators, and recursive algorithms. This enables efficient internal coordinate molecular dynamics simulation for the modelling of protein structures.

Date: Feb. 15 (Mon.), 2016

Time: 2:00 pm – 4:00 pm

Place: A3-024, Katsura Campus

※この講演は、「物質機能・変換科学分野」のSGU群科目「JGPセミナーI ～ III」の単位認定対象講演となります。詳細は、JGP化学系オフィス（090jgpchem@mail2.adm.kyoto-u.ac.jp）にお問い合わせ下さい。

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