

□第19回 MaDIS研究交流会&第87回 構造材料ゼミ

OPEN SEMINAR SERIES & The 87th Structural Materials Seminar

2018 **5.15** Tues.

Open 14:00-16:00

#2 Conference Room,
Main Bldg., Sengen, NIMS

Assistant Prof. Dr. N.S.Venkataramanan

(SASTRA Deemed University)

Title: Deciphering the selective recognition of
nutraceuticals by supramolecules



Abstract:

Developing safe, and nontoxic drug carriers for nutraceuticals is essential to increase their bio-availability in the human body. Supramolecules such as cyclodextrin, cucurbit[*n*]uril and pillar[*n*]anes are capable of forming inclusion complexes with drugs. In this talk, the complex formation ability of supramolecules with nutraceuticals and drugs will be discussed. The formation of host-guest complexes was first studied using various spectroscopic techniques. Deciphering nature of the interaction between the host supramolecule and the guest molecules would result in improving the materials property. To obtain the atomistic information, density functional theory combined with atoms-in-molecules analysis were carried out. Energy decomposition and noncovalent interaction analysis has been performed to understand the nature of interactions in the host-guest complexes.



Prof. Dr. Prasenjit Ghosh

(Indian Institute of Science Education and Research (IISER) Pune)

Title: Atomistic modeling of materials

Abstract:

In this talk I will briefly discuss the ongoing research activities in my group where we primarily use density functional theory (and its variants) based simulations to (a) understand aspects of chemical bonding and microscopic couplings that are essential to specific property of materials, (b) obtain atomistic information and electronic states which are often hard and sometimes inaccessible to experiments and (c) design new materials and /or modify existing materials to obtain desired property.

Coordinator :

Dr. Ryoji SAHARA,

Dr. S. K. BHATTACHARYA

(Research Center for Structural Materials)

Contact address : madis@ml.nims.go.jp



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NIMS MATERIALS DATA and
INTEGRATED SYSTEM

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Research Center for Structural Materials