materials science &ENGINEERING

1st Symposium on

Computational Materials Research

Advanced Electronic Structure Calculations and Big Data

Thursday July 27, 2017 9am - 4pm IMS 20, UConn Storrs Campus*

SYMPOSIUM SCOPE

Quantum theory has been at the forefront of materials research as the technology shrinks towards the nanoscale. This has been partly driven by the progress in methodologies that could be pursued within present day high-performance computational capabilities. The state-of-the-art theory goes hand-in-hand with experiments and helps capture the physics of materials. There are examples where new properties predicted by theory have been later validated by experiments. The data mining and the machine learning of the first-principles data adds completely new dimension to designing materials by theory. The goal of the conference is to provide a platform for discussion on the current research trends. The scope also covers some introductory and visionary perspective in materials theory.


S. Pamir Alpay


S. Rajasekharan


Sanjubala Sahoo


Huan Tran


Deya Das


Sanjeev K. Nayak


Lydie Louis


Anand Chandrasekharan


Chiho Kim

TOPICS

- Density Functional Theory (DFT), its Advantage and Limitations
- Wannier Functions and their Applications
- Phonons and their Properties
- Applications of DFT for Physical and Catalytic Properties
- Data Mining and Machine Learning

APPLICABLE FOR

- Graduate students
  (Materials Science and Engineering, Physics, Chemistry)
- Industry researchers interested in brushing up theory knowledge
- IMS/MSE Postdocs
- Faculty members (IMS, MSE, Physics, Chemistry)

REGISTRATION

Deadline **July 20, 2017** (no fee)

For further information, contact
Dr. Sanjeev K. Nayak (*sanjeev.nayak@uconn.edu*)

SPEAKERS

IMS Postdoctoral Members
Keynote Speaker: S. Rajasekaran, UConn Professor & BECAT Director

UCONN SCHOOL OF ENGINEERING

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MRS MATERIALS RESEARCH SOCIETY

IMS INSTITUTE OF MATERIALS SCIENCE

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