



Tokyo Tech



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Tokyo Institute of Technology and Uppsala University Joint Workshop Theoretical and Computational Approach to New Materials

元素戦略研究センター（MCES）では6月4日(木)と5日(金)の2日間にわたり、表記合同 Workshop を開催いたしました。東京工業大学と Uppsala 大学（Sweden）とは昨年来、教育・研究における交流を深めており、今回の Workshop はその一環として行われました。Uppsala 大学は材料計算、計算機支援材料設計などに強みを持ちます。これは MCES における材料研究の方向性に合致しており、本 Workshop の実現に至りました。

4日は約50名の参加者を集め、安藤真理事・副学長（研究担当）の開会挨拶に続き、Uppsala 大学 Senior Professor である Claes-Göran Granqvist による Uppsala 大学の紹介、当該分野における国際的研究者である Kee Joo Chang (KAIST)、John Robertson (Cambridge Univ.)による特別講演が行われました。午後からは東工大より4名、Uppsala 大より2名の招待講演が行われ、熱心な議論が交わされました。5日は約50名の参加者を集め、Discussion Day と銘打った討論中心の Workshop が展開されました。東工大はじめ6名の日本側若手研究者が15分程度のトピックス提供を行い、これに関し参加者が討論するという形で進行しました。前日にもまして熱い議論が闘わされました。

Date: 10:00-19:00, 4th June, 2015: Lecture Session
10:00-16:00, 5th June, 2015: Discussion Session

Venue: Lecture Hall in Genso cube

Organized by

Tokyo Institute of Technology and Uppsala University

Co-organized by

Materials Research Center for Element Strategy
Tokodai Institute of Element Strategy sponsored by MEXT
ACCEL Hosono Electride Project by sponsored by JST

Endorsed by

Materials Engineering Committee of Science Council of Japan



Program

4th June: Lecture Day

Opening Remarks

Makoto Ando (Vice-President of Tokyo Institute of Technology)

Key-note Lecture (chairperson: Hideo Hosono)

Claes-Göran Granqvist (Uppsala University, Sweden)

Uppsala University: Old and New

Plenary Lecture (chairperson: Hideo Hosono)

Kee Joo Chang (Korea Advanced Institute of Science and Technology, Korea)

First-principles materials design via an inverse method based on conformational space annealing

John Robertson (University of Cambridge,



Claes-Göran Granqvist



Kee Joo Chang



John Robertson

UK)

Computational Design of new Electronic Functional Materials

Invited Lecture (chairperson: Tomofumi Tada and Susumu Saito)

Tomas Edvinsson (Uppsala University, Sweden)

Theoretical Calculations of Energy Relevant Materials - Towards Time Resolved Relativistic Quantum Mechanics in Materials Science

Susumu Saito (Tokyo Institute of Technology, Japan)

Designing Materials for Electronics using B, C, and N

Shuichi Murakami (Tokyo Institute of Technology, Japan)

Weyl-semimetallic phase and chiral transport in chiral crystals



Tomas Edvinsson



Susumu Saito



Shuichi Murakami

Biplab Sanyal (Uppsala University, Sweden)

Electronic structure of correlated electron systems by ab initio theory

Fumiyasu Oba (Tokyo Institute of Technology, Japan)

Accurate predictions of defect properties in semiconductors:
Towards understanding and screening of materials

Tomofumi Tada (Tokyo Institute of Technology, Japan)

High-throughput ab initio modeling for two-dimensional electrider materials



Biplab Sanyal



Fumiyasu Oba



Tomofumi



5th June: Discussion Day

(Chairperson: Tomofumi Tada and Satoru Matsuishi)

40 min per 1 topic (topic presentation 15 min + discussion 25 min)

Topic presenter (random order)

Satoru Matsuishi (Tokyo Institute of Technology, Japan)

Hydride ion substitution to oxides and related compounds

Soshi Iimura (Tokyo Institute of Technology, Japan)

Syntheses and physical properties of iron-based superconductors $\text{LnFeAsO}_{1-x}\text{H}_x$

Zewen Xiao (Tokyo Institute of Technology, Japan)

Electronic Structure and Native Defects of Air-Stable and Lead-Free Perovskite Variant Cs_2SnI_6 for Photovoltaic Application

Naoki Ohashi (National Institute of Materials Science, Japan)

Hard-x-ray photoemission in terms of crystalline polarity and x-ray polarization

Keiji Kojima (High Energy Accelerator Research Organization, Japan)

Bipartite magnetic parent phases in the iron oxypnictide superconductor

Taisuke Ozaki (The University of Tokyo, Japan)

Open source package OpenMX for first-principles electronic structure calculations



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