

【Symposium title】

The 1st International Symposium on Novel Materials for Next Generation Electronics and Catalysis

【Date and time】

February 16 (Thu), 2017, 09:00-17:55

(reception: 18:20-19:40)

February 17 (Fri), 2017, 09:00-15:15

【Symposium site】

Lecture Hall, 1F of Genso-Cube (S8 building), Suzukakedai campus,
Tokyo Tech

【Program】

Please see the following page.

【Reception】

Date and time: February 16 (Thur), 2017, 18:20-19:40

Place: Party space, 3F of H1 & H2 Bldgs., No. 25 of

<http://www.titech.ac.jp/english/maps/suzukakedai/index.html>

Contribution fee: 4,000 JPY

【Contact information】

Please fill out the following Attendance inquiry and e-mail it to ties@lucid.msl.titech.ac.jp

※Deadline February 9 (Thu)

<Attendance inquiry>

- Your name:
- Your affiliation:
- Attendance to the symposium(Feb.16): YES/NO
- Attendance to the symposium(Feb.17): YES/NO
- Attendance to the reception: YES/NO

<Program>

February 16, Thursday, 09:00-17:55

09:00-09:20 Opening Remarks

Hideo Hosono (Tokyo Tech)

1. Technical Session on computational approaches I

Chaired by Peter V. Sushko (PNNL)

1.1. 09:20-09:55

Electron and hole trapping in amorphous oxides

Alex Shluger (UCL)

1.2. 09:55-10:30

In silico design and exploration of novel semiconductors

Fumiyasu Oba (Tokyo Tech)

Break 10:30-10:45

1.3. 10:45-11:20

Computational materials design for renewable energy applications

David Scanlon (UCL)

1.4. 11:20-11:55

Theoretical aspects of topological materials from *ab initio* calculations

Motoaki Hirayama (Tokyo Tech)

Lunch 11:55-13:00

2. Technical Session on computational approaches II

Chaired by Fumiyasu Oba (Tokyo Tech)

2.1. 13:00-13:35

Catalytic function activated by localized electrons and hydrogen transfer

Peter V. Sushko (PNNL)

2.2. 13:35-14:10

New strategy on first principles and evolutionary computations for electrides

Tomofumi Tada (Tokyo Tech)

2.3. 14:10-14:45

Atomistic modeling of porous catalysts

Ben Slater (UCL)

2.4. 14:45-15:20

Density-functional approaches to two-dimensional materials

Susumu Saito (Tokyo Tech)

Break 15:20-15:35

3. Technical Session on s semiconductors, superconductors, and dielectrics I
Chaired by Hiroshi Funakubo (Tokyo Tech)

3.1. 15:35-16:10

Chemical-vapor deposition of oxide semiconductors

Ivan Parkin (UCL)

3.2. 16:10-16:45

Control of defects to develop new amorphous oxide semiconductors

Toshio Kamiya (Tokyo Tech)

3.3. 16:45-17:20

Sustainable, continuous hydrothermal production of advanced functional nanomaterials; from lab to pilot plant

Jawwad Darr (UCL)

3.4. 17:20-17:55

Heteroepitaxial growth and electric field-induced phase transition of layered iron-selenides

Hidenori Hiramatsu (Tokyo Tech)

Reception 18:20-19:40

February 17, Friday, 09:00-15:15

4. Technical Session on semiconductors, superconductors, and dielectrics II
Chaired by Ivan Parkin (UCL)

4.1. 09:00-09:35

Understanding the activity of tungsten oxide nanostructures for photon-driven applications

Chris Blackman (UCL)

4.2. 09:35-10:10

Heteroepitaxy of functional materials for environmental and energy applications

Akira Ohtomo (Tokyo Tech)

4.3. 10:10-10:45

Precursor Synthesis for CVD of TCOs and Metals

Caroline Knapp (UCL)

Break 10:45-11:00

4.4. 11:00-11:35

Ferroelectric and dielectric materials for power electronics and automobile applications

Hiroshi Funakubo (TokyoTech)

5. Technical Session on catalytic and related materials

Chaired by Tomofumi Tada (Tokyo Tech)

5.1. 11:35-12:10

Real-time catalyst characterization under reaction conditions

Andrew Beale (UCL)

Lunch 12:10-13:10

5.2. 13:10-13:45

Electride catalysts for ammonia synthesis and chemical reactions

Masaaki Kitano (Tokyo Tech)

5.3. 13:45-14:20

Structure of dopants in Catalysts and transparent conducting oxides

Gopinathan Sankar (UCL)

5.4. 14:20-14:55

High-pressure synthesis of oxyhydrides and related compounds

Satoru Matsuishi (Tokyo Tech)

6. 14:55-15:15 Concluding Remarks

Alex Shluger (UCL)