

**Uppsala-Osaka mini-workshop on Computational Materials Design
May 4, 2015**

Å80101

9:30 – 10:00 **Hiroshi Katayama-Yoshida**, *Computational nano-materials design for self-regenerated and self-organized photovoltaic solar cells: design vs. realization*

10:00 – 10:30 **Barbara Brena** *Ab initio Modeling of Soft X-ray Spectra for Solar Energy Applications*

10:30 – 11:00 **Coffee**

11:00 – 11:30 **Biplab Sanyal**, *Electron correlation in functional metalorganics by density functional theory and exact diagonalization*

11:30 – 12:00 **Hisazumi Akai**, *Reformulation of optimized effective potential method and its application to RPA level correlation*

12:00 – 13:30 **Lunch**

Polhemsalen

13:30 – 14:00 **Tamio Oguchi**, *Exploration of cathode materials for sodium batteries*

14:00 – 14:15 **Mikhail Poluektov** *Multiscale modeling*

14:15 – 14:30 **Alexander Edström**, *Computational design of permanent magnets*

14:30 – 15:00 **Kazunori Sato**, *Clustering and ferromagnetism in magnetic semiconductors*

15:00 – 15:30 **Coffee**

15:30 – 16:00 **Yaroslav Kvashnin** *Magnetic materials and their ground state stability from first-principles*

16:00 – 16:30 **Manuel Pereiro**, *Topological excitations in a kagome magnet*

16:30 – 17:30 *Round-table discussion on future plan towards "Computational Materials Design on Green energy"* (conducted by Katayama-Yoshida and Eriksson)

18:30 – 21:00 **Dinner**