

未来研究イニシアティブ
「計算機ナノマテリアルデザイン新元素戦略」
1 DAY SYMPOSIUM

January 26th, 2015
基礎工学研究科シグマホール／セミナー室

Session 1:

- 10:00 – 10:20 (20 min.) 吉田 博 (阪大基礎工)
Computational materials design of negative effective U for super-high- T_c superconductor
- 10:20 – 10:40 (20 min.) 真砂 啓 (阪大基礎工)
Theoretical Approach to Local Contact Potential Difference in Kelvin Probe Force Microscopy
- 10:40 – 11:00 (20 min.) 植本 光治 (阪大基礎工)
Large and well-defined Rabi splitting in semiconducting nanodimer.
- 11:00 – 11:10 (10 min.) 休憩 (break)

Session 2:

- 11:10 – 11:30 (20 min.) 船島 洋紀 (阪大基礎工)
Theoretical Study of Half-Heusler Alloy as Thermoelectric Materials
- 11:30 – 11:50 (20 min.) Mohammad Hussein Naseef Al Assadi (阪大基礎工)
Ab Initio Insight into the Spin Entropy and the Transport Phenomena in Thermoelectric Na_xCoO_2
- 11:50 – 12:10 (20 min.) 山内 邦彦 (阪大産研)
A long-standing mystery about magnetite: the charge and orbital orderings
- 12:10 – 13:00 (50 min.) lunch break

Session 3: 固体物理セミナー

- 13:00 – 14:30 (90 min.) Peter H. Dederichs (FZJ, Juelich)
Friedel Oscillations - In the Bulk and on Surfaces
- 14:30 – 14:40 (10 min.) 休憩 (break)

Session 4:

- 14:40 – 15:10 (30 min.) 赤井 久純 (東大物性研)
Going beyond LDA
- 15:10 – 15:40 (30 min.) 小谷 岳生 (鳥取大)
QSGW calculations and Wannier function analysis for La_2CuO_4 and related cuprates.
- 15:40 – 15:50 (10 min.) 休憩 (break)

Session 5:

- 15:50 – 16:10 (20 min.) 靱田 浩義 (阪大産研)
First-principles study of reaction mechanism in sodium batteries
- 16:10 – 16:30 (20 min.) 豊田 雅之 (阪大産研)
A-site magnetic ordering in quadruple perovskite oxides
- 16:30 – 16:50 (20 min.) 藤井 将 (Spring-8)
X-ray magnetic circular dichroism at Re L-edge in A- and B-site ordered perovskite
 $\text{CaCu}_3\text{Fe}_2\text{Re}_2\text{O}_{12}$
- 16:50 – 17:10 (20 min.) 鈴木 通人 (理研)
First-principles theory for orbital ordered states in f-electron compounds
~Application of LDA+U method to multipole ordered states~
- 18:00 – 20:00 意見交換会 (みのお山荘、風の杜)
- 世話人： 小口 多美夫 (阪大産研)
佐藤 和則 (阪大工)
福島 鉄也 (阪大基礎工)
- 20:00 – 21:00 3 拠点連携会議
赤井久純 (東大物性研)
Peter H. Dederichs (FZJ, Juelich)
世話人： 吉田 博 (阪大基礎工)