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Joint Seminar 2016 (第 9 回材料構造講演会)

参加費:無料

 $12:45\sim$

日時:2016年7月19日(火曜日) 場所:すずかけホール2F 集会室1

[PROGRAM]

(座長 東工大 安井伸太郎)

$12 \cdot 50 \sim$	Li ₂ CO ₃ と CoO の焼結反応を用いたエピタキシャル LiCoO ₂ 薄膜の

PLD 合成 (東北大 丸山伸伍)

Opening remarks

13:05~ 成長温度がスピネルとナノ相分離した Bi 層状ペロブスカイトの安定

性に及ぼす影響(東北大 原田龍馬)

13:20~ パルスレーザー液相エピタキシーによる Si-Ge 系融液を用いた 3C-SiC ヘテロエピタキシャル成長の試み (東北大 山王堂尚輝)

13:35~ 第一原理計算を用いた未開拓物質群の開拓 (NIMS 大久保勇男)

13:50~ 酸化物ヘテロ界面・表面の酸素配位環境の制御と機能 (京都大 菅大介)

14:05~ シーメンス法応用へ向けた、熱フィラメント法による大気圧での水素 ラジカルの生成 (筑波大 岡本裕二)

14:20~ リチウム電池正極材の Ti 置換効果 (東京理科大 藤本憲次郎)

14:35~ Coffee break (25 分)

(座長 東北大 丸山伸伍)

- 15:00∼ Holographic analysis of dopant site structure in perovskites (Univ. Tokyo Mikk Lippmaa)
- 15:15~ ナノコンンポジット構造を持つ水分解光電極 (東京大 高橋竜太)
- 15:30~ Crystal structure and electronic status of substituted halide perovskites based on density functional calculation and molecular dynamics (Kogakuin Univ. Md. Alam Khorshed)
- 15:45~ ペロブスカイト/Si タンデム型太陽電池開発の コンビナトリアル デバイス作製プロセスによる高速化 (神奈川大 松木伸行)
- 16:00~ 有機無機ハイブリッド積層膜のコンビナトリアル分子層製膜システム とハライドペロブスカイト材料開発への応用 ((株)コメット 川嶋 一裕)
- 16:15~ Break (15分)

(座長 東京大 高橋竜太)

16:30~ ~ Special Invited Talk-1~ $(30 \, \%)$

Smart materials for cooling and energy harvesting (Université de Lyon, Gael Sebald)

Abstract: First, the lab ELyTMaX located in Tohoku University will be introduced. It is a joint French-Japan laboratory created by Université de Lyon, CNRS and Tohoku University. One personal example of recent collaboration between Lyon and Tohoku will be presented, dealing with magnetorheological elastomers for energy harvesting. The characterization of the elastomers, as well as an estimation of energy conversion capability will be given. Another research topic will then be presented, and deals with electrocaloric and elastocaloric properties, based on former work held at LGEF lab from INSA-Lyon. In these materials, the entropy is a function of an external quality (electric field or mechanical strain), and the implication on internal energy variation is discussed.

17:00~ ~ Special Invited Talk-2~ (45 分)

Machine learning for combinatorial materials science (Univ. Maryland, Ichiro Takeuchi)

Abstract: We have been applying machine learning techniques for rapid analysis of combinatorial library data. In particular, we have been looking at various clustering algorithms for x-ray diffraction data, so that we can quickly determine the distribution of structural phases across composition spreads. I will discuss our latest work where we performed critical comparison of different metrics used for clustering of diffraction data based on accuracy and computational cost. We have identified the best combination of algorithms which are applicable for all X-ray diffraction data. I will also discuss our recent active learning exercises where we let the computer dictate how characterization of libraries is carried out.

17:45 Closing

18:00~ Banquet (モトテカコーヒー すずかけホール 2 階) 会費 5000 円 (学生 3000 円)