東京理科大学　マテリアルズインフォマティクス懇談会

第4回研究会

2019年11月1日(金)　13時より

於 ： 森戸記念館　第二フォーラム

参加費 ： 無料

材料科学と情報科学を融合するマテリアルズインフォマティクス(MI)の研究開発が本格化しています。 第4回となるTUSMI懇談会では､MI研究の最前線を共有すべく、サウサンプトン大学のBrian Hayden教授より講演いただきます。また、本学で取り組んでいるMIの研究開発について紹介します。

13:00　趣旨説明　東京理科大学(TUS)　藤本憲次郎

基調講演

13:05　サウサンプトン大学　Brian Hayden
「Materials Development in the Energy and Electronics Sectors through Combinatorial Synthesis, High-Throughput Screening and Machine Learning」

一般講演

14:05　東京理科大学(TUS)　小嗣真人
「非負値行列因子分解による顕微分光データのクラスタリング」

休憩(15分)

15:00　名古屋大学　山崎 貴大
「センサ応用に向けた磁歪材料のバルクハウゼンノイズ解析」

15:40　東京理科大学(TUS)　Alexandre Lila Foggiatto
「The relation between morphology and electrical properties in organic semiconductors」

ジュニアセッション

16:20　東京理科大学(TUS)　西尾直
「鉄系合金薄膜の磁気相転移現象のハイスループット解析」

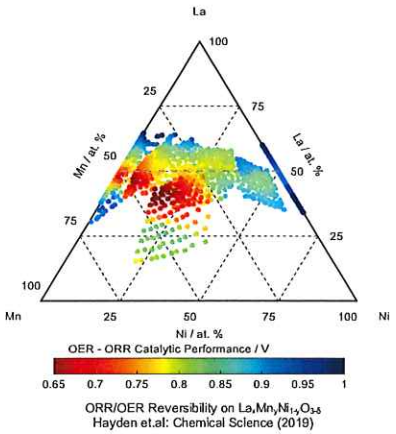
16:45　まとめ　東京理科大学(TUS)　小嗣真人

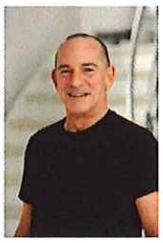
Materials Development in the Energy and Electronics Sectors through Combinatorial Synthesis, High-Throughput Screening and Machine Learning

Brian E Hayden

Chemistry, University of Southampton, SO17 1BJ, UK.

The combinatorial synthesis of solid-state materials combined with high-throughput characterization and screening provides an opportunity to develop increasingly large materials data-bases, with the ultimate goal of understanding the function/composition/structure relationship, and ultimately to predict and confirm the function of new materials. There have been several approaches taken centred on combinatorial thin film synthesis of materials, however a step change in the development of new functional materials has taken place with the introduction of combinatorial evaporative PVD (ePVD) synthesis. The advantages of the approach are exemplified in combinatorial studies of solid solution in perovskite oxides, and in metal alloys. Imbedded in the associated informatics, machine learning approaches are crucial in aspects of the building, interpretation and exploitation of such data-bases, which can ultimately include physical and chemical descriptors from, for example, ab-initio calculation. The challenge is to ensure an audited content and consistent format of the experimental data. Examples of how machine learning is being developed in the interpretation of raw data sets is presented using data from high throughput investigations of perovskite electrocatalysts mediating the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) for the development of reversible fuel cells and rechargeable metal-air batteries. The use of neural-networks in the interpretation of perovskite lithium ion conductors for solid state batteries is also presented. The results provide an insight into the potential opportunities of machine learning in the future in the predictive development of functional materials.





Brian Hayden FRSC FIoP is Professor of Chemistry at the University of Southampton and director of the Advanced Composite Materials Facility dedicated to combinatorial materials discovery and their incorporation into devices, through evaporative PVD methods on a 150mm wafer scale. He is a founder (2004), an executive director and Chief Scientific Officer of Ilika plc, a £50M spin-out company involved in materials discovery and development for the electronics and energy sectors, and with strong partnerships with multinational corporations. His present research interests include the development of fuel cell electrocatalysts, materials in solid state lithium ion batteries, optoelectronic and metamaterials and tunable dielectric materials for 5G applications. He is author of over 150 refereed papers {h-index 39} and over 30 active patent families including catalysts for PEMFC and materials for solid state Li-ion batteries.