第292回応用セラミックス研究所講演会
292nd MSL Lecture

Date/Time: 15:00-16:00, Friday, June 19th

Venue: 1F Meeting Room, Building R3

Speaker: Dr. Keith Butler

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Title: Computer-aided materials design: Electronic insights and chemical knowledge in the quest for functionality

Abstract:

The advent of new technology has vastly increased the power of computation for the simulation of the most fundamental properties of matter. At the same time the demand for new technology has increased the need for the discovery of new materials and the re-investigation of hitherto overlooked ones. For the latter task, high-throughput screening enterprises such as Materials Project and the OQMD are well suited to the application of density functional theory for assessing the merits of known materials. The former task, however, necessitates the exploration of novel combinations of atoms and molecules. The blind exploration of the combinations and permutations of the periodic table is a daunting task, to paraphrase Samuel Beckett we feel *lost before the confusion of innumerable prospects*.

Centuries of chemical research have provided us with myriad rules for assessing the feasibility of a given stoichiometry and the likelihood of particular crystal arrangements. In this presentation I will explore the ways in which chemical knowledge and state-of-the-art computational physics can be combined to accelerate materials design. I will introduce the SMACT (Semiconducting Materials by Analogy and Chemical Theory) package, which combines these chemical rules with combinatorial searching of chemical space to predict plausible and heretofore unknown compounds.

I will then provide some illustrative examples of materials' design focusing on several important issues: (i) designing new photovoltaic materials [1], (ii) the role of surfaces and polymorphism in controlling electronic properties [2-4], (iii) going beyond the condensed phase, the design of porous materials [5,6] and (iv) going beyond crystal structures, understanding and predicting the properties of amorphous materials [7].

[1] K. T. Butler, J. M. Frost, and A. Walsh, *Energy Environ. Sci.*, **2015**, 8, 838
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[3] J. Buckeridge, K. T .Butler, C. R. A. Catlow, A. J. Logsdail, D. O. Scanlon, S. A. Shevlin, S. M. Woodley, A. A. Sokol, A. Walsh, *Chem. Mater.*, **2015**, 27, 3844
[4] K. T. Butler, *Phys. Stat. Sol. (a)* **2015** DOI: 10.1002/pssa.201532004
[5] K. T. Butler, C. H. Hendon, A. Walsh, *J. Am. Chem. Soc.*, **2014**, 136, 2703
[6] K. T. Butler, C. H. Hendon, A. Walsh, *ACS Appl. Mater. Interfaces*, **2014**, 6, 22044
[7] S. Sallis, K. T. Butler, N. F. Quackenbush, D. S. Williams, M. Junda, D. A. Fischer, J. C. Woicik, N. J. Podraza, B. E. White Jr, A. Walsh, L. F. J. Piper, *Appl. Phys. Lett.,* **2014**, 104, 232108

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