High throughput computation of all inorganic materials

Daniel W. Davies[1], Adam J. Jackson[1], Keith T. Butler[1], Andrew Morris[1], Jonathan M. Skelton[1], Jarvist M. Frost[1] and Aron Walsh[1,2]
[1]*Centre for Sustainable Chemical Technologies and Department of Chemistry, University of Bath, Claverton Down, Bath, BA2 7AY, UK;* [2]*Global E*^{3} *Institute and Department of Materials Science and Engineering, Yonsei University, Seoul 120-749, Korea*
E-mail: d.w.davies@bath.ac.uk

Over the past decade, high-throughput computational screening projects have exploited the power of modern computers in order to assess and compare known bulk materials using high level electronic structure theory. The Materials Project, for example, has performed calculations on over 66,000 compounds[1,2] in order to help accelerate the process of materials discovery. But what fraction of chemical space does the number of known compounds analysed by this and similar enterprises represent? The task of exploring new combinations of the periodic table is a daunting one; forming a four component compound from the first 103 elements results in excess of 10^{12} potential combinations. Such materials space is intractable to high-throughput experiment or first-principles computation and in order to tame this combinatorial explosion we can turn instead to an arsenal of rules that are the product of centuries of research.

We present the open-source SMACT (Semiconducting Materials by Analogy and Chemical Theory) package,[3] which implements simple chemical constraints in the search through materials space in order to remove implausible compounds. We show how well-established chemical knowledge, such as the concept of electronegativity as defined by Mulliken,[4] can be used alongside other heuristically derived data such as those in Harrison's Solid State Table of the Elements[5] and the more recent Solid State Energy Scale as proposed by Pelatt *et al.*[6] to estimate key properties of chemical compositions such as band gaps and absolute electron energies. Crucially, these estimations can be made even before considering structure. We illustrate this methodology in the search for: a) binary transparent conductors and b) new ternary chalcohalide materials for use as photoelectrodes for water splitting. Finally, we demonstrate the applicability of this approach to structure prediction by assessing possible ternary combinations of elements that satisfy the radius ratio rule to form a perovskite lattice.

Bibliography

[1] http://www.materialsproject.org (Accessed 01.04.16).
[2] A. Jain, S. P. Ong, G. Hautier, W. Chen, W. D. Richards, S. Dacek, S. Cholia, D. Gunter, D. Skinner, G. Ceder and K. A. Persson, *APL Mat.*, **1**, 011002 **(2013)**
[3] http://www.github.com/WMD-group/SMACT
[4] R. S. Mulliken, *J. Chem. Phys.,* **2**, 782 **(1934)**
[5] W.A. Harrison, *Electronic Structure and the Properties of Solids,* Dover Publications Inc., New York **(1980)**
[6] B. D. Pelatt, R. Ravichandran, J. F. Wager, D. A. Keszler, *J. Am. Chem. Soc.*, **133**, 16852 **(2011)**