Design of Advanced Materials?

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The knowledge we have developed through the synthesis and experimental study of extended solids allows us to efficiently identify new materials, in many cases with scientifically interesting or technically important changes in properties. An example is the chemical control of the transparent conducting behaviour of correlated metals (1), evaluated as epitaxial films through optical and transport data. The selection of d^0 cations to stabilise oxygen-oxygen bond formation upon deep oxidation of lithium ion cathodes is a further example (2). Here computation provides underpinning guidance in the selection of experimental targets.

However, the large potential range of accessible compositions and structures challenges our present capabilities. As part of the current interest in exploring computationally-enabled routes to new materials, we are developing computational tools for the identification of stable new compositions. We have recently (3) been able to predict *ab initio* the regions of composition space that afford new materials, and then subsequently isolate those materials experimentally, using the computation of the energies of probe structures identified by new crystal structure prediction methods (4) to explore the space. The presentation will discuss the potential offered by informatics approaches often referred to as machine learning in such work.

(1) J.L. Stoner *et al.*, *Advanced Functional Materials* **29**, 1808609, 2019

(2) Z. Taylor et al., *J. Am. Chem. Soc.* **141**, 7333, 2019

(3) C. Collins *et al., Nature* **546**, 280-284, 2017

(4) C. Collins *et al.*, *Faraday Discussions* **211**, 117, 2018