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Simple Rules for Solid-state Design: From Bulk to Interface KEITH BUTLER, ARON WALSH, ADAM JACKSON, DAN DAVIES, University of Bath, FUMIYASU OBA, YU KUMAGAI, Tokyo Institute of Technology, WALSH MATERIALS DESIGN TEAM, JSPS COLLABORATION — 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 bulk materials. The blind exploration of the new 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 research have provided us with myriad rules for assessing the feasibility of a given stoichiometry and the likelihood of particular crystal arrangements. We explore the ways in which chemical knowledge and state-of-the-art computational physics can be combined to accelerate materials design. We present the SMACT (Semiconducting Materials by Analogy and Chemical Theory) package, which combines these rules with 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 [2,3], and (iii) the design of porous materials [4]. [1] K. T. Butler et al., *Energy Environ. Sci.*, **2015**, 8, 838 [2] K T. Butler et al., *Phys. Rev. B*, **2014**, 89, 115320 [3] J. Buckeridge, et al., *Chem. Mater.*, **2015**, 27, 3844 [4] K. T. Butler, et al., *J. Am. Chem. Soc.*, **2014**, 136, 2703

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