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**First Principles Modelling Insights into Lithium-Ion Battery Materials including Point Defects.** ANDREW MORRIS, CLARE GREY, CHRIS PICKARD, MARTIN MAYO, KENT GRIFFITH, University of Cambridge — The traditional lithium-ion battery(LIB) anode is composed of graphite but recently silicon has been proposed as an alternative due to its ten-fold increase in theoretical capacity. Using AIRSS[1] we have predicted phases of lithium group 4, group 5 and group 6 compounds[2,3,4] finding many new phases. We calculate average voltages, capacities and chemical shielding and compare these with in situ and ex situ NMR and XRD experiments[4,5]. Point-defect impurities can dramatically alter the properties of these materials. I show how using the defect-AIRSS technique we can obtain an insight into such processes in LIB, presenting some impurities which mitigate[6,7] and some which augment a battery's function[5].

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