Computational studies of V_2O_5 and TiO_2 as cathode materials for Mg ion batteries

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The development of cathode materials using earth abundant materials and offering suitable operating voltages, long cycle life and good kinetics is a crucial step towards Mg-ion battery technology that can provide performance advantages over Li-ion technology. Here we present our computational studies of two Mg-ion battery cathode materials that could fulfil these criteria: V_2O_5 and TiO_2.

Orthorhombic α-V_2O_5 demonstrates reversible Mg intercalation at an average voltage of ~2.5 V and has a good theoretical capacity of ~300 mA h g^{-1}, however it suffers from several performance issues, the most critical of which is limited kinetics. Experimental results indicate that doping can be used to improve electrochemical performance for V_2O_5 as a Li ion cathode material,[1] and we speculate that similar improvements may be achieved by doping in the $Mg_xV_2O_5$ system. Here we present computational results investigating the location and effects of a range of metal ion dopants in α-V_2O_5, the factors affecting the stability of the important α- and δ- phases, and how doping can be tailored to modify Mg mobility.[2]

TiO_2 is an attractive sustainable material for battery applications and has a theoretical capacity of ~ 290 mA h g^{-1} for Mg storage, yet experimental capacity is limited to ~40 mA h g^{-1}. We use DFT to unravel the mechanisms that contribute to this low performance and how they may be overcome using rationally designed doping strategies.

References

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