Defects and Ion Transport in Materials with the $Sc_2(WO_4)_3$ Type Structure

Daniel J. Driscoll, M. Saiful Islam and Peter R. Slater

Department of Chemistry,
University of Surrey,
Guildford, GU2 7XH
Email: D.Driscoll@surrey.ac.uk

Materials with the $Sc_2(WO_4)_3$ structure have attracted considerable interest due to them exhibiting trivalent cation conduction [1] and negative thermal expansion [2]. The structure consists of Sc−O octahedra corner sharing with W−O tetrahedra to create an open framework. Computer simulation techniques have been successfully employed to model the complex structure of $Sc_2(WO_4)_3$. The results indicate a good agreement between the simulated and experimental structures. The energetics of ionic defects have also been calculated, resulting in high intrinsic defect energies. Energetics of dopant incorporation have also been investigated with isovalent doping on the Sc site being generally energetically favourable. Experimental doping studies have confirmed the latter, and have also shown the material to be resistant to doping strategies directed at the incorporation of either Sc vacancies or interstitials.

1. Kohler J., Imanaka N., Adachi G., *J. Mater. Chem.* **9** (1999) 1357
2. Evans J.S.O., Mary T.A., Sleight A.W., *J. Solid State Chem.* **137** (1998) 148