Computational prediction and experimental confirmation of electronic and optical properties of transition metal substituted $A_2B_2O_7$ structures

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Presentation Preference: Oral (can also be Poster)

Career Level: Early Career Scientist (<5 yrs post PhD)

Aligned with Science Focus: Photo-catalysis

Abstract:

The electronic properties and crystal structures of $Bi_{1.5}CdM_{1.5}O_7$ (M = Nb, Ta) pyrochlores have been investigated using computational Density Functional Theory (DFT) and experimental analyses, including ultraviolet-visible (UV-Vis) spectrometry, X-ray diffraction (XRD), Raman spectroscopy and transmission electron microscopy (TEM). Computationally predicted results on electronic and crystal structures suggest that specific site Cd-cation substitutions (particularly in the *B*-site of the crystal structures) are required to obtain electronic band gaps in the calculated energy band structures, when using the Full Plane Waves Functions in DFT calculations. Differences in calculated enthalpies are substantial and support ordered substitutions at preferential sites, rather than random distribution of transition metals suggested by initially investigated structures from the crystallographic information files (CIF). DFT calculated band gaps are in excellent agreement with estimated values from optical absorption measurements, particularly for $Bi_{1.5}CdTa_{1.5}O_7$. In addition to the prediction of electronic structures, the models also indicate that the large ionic radius of the Cd-cation leads to symmetry modification from the archetypal cubic pyrochlore structure in $Bi_{1.5}CdM_{1.5}O_7$ (M = Nb, Ta) pyrochlores, although the cation size ratios, r_A/r_B, are within cubic symmetry range (1.46 - 1.78). Rhombohedral structures and localized superlattice order are confirmed using comprehensive analytical techniques. (196 words)

Biographical Statement of speaker:

Dr. Ganchimeg Perenlei received her Ph.D from Queensland University of technology (QUT) in 2015. Currently she is working as a research assistant at QUT. Her research interests are mainly on synthesis and characterization of new complex metal oxide nanomaterials for energy conversion and storage applications using theoretical and experimental approaches. (50 words)