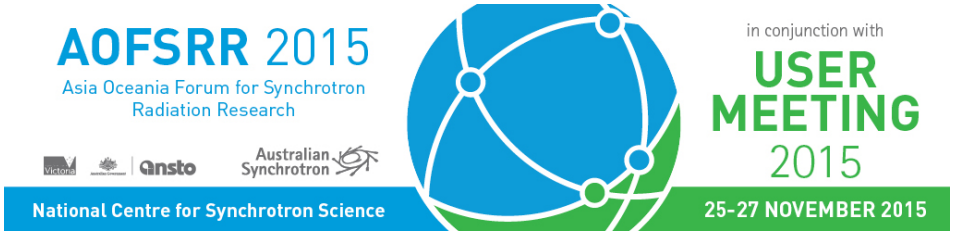

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Synchrotron XPS, EXAFS and IR studies of atomically precise chemically made clusters

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We are exploring the use of atomically-precise, chemically-synthesised metal clusters deposited on various forms of oxides with a view to understanding how and why they perform as catalysts and sensors.1, 2 Although measurement of their catalytic activity is important, it is vital to identify and understand the geometric and electronic structure of the active sites to make further gains in photocatalytic efficiency and efficacy. Consequently, theoretical modelling on atomically precise co-catalysts can provide understanding to interpret and explain experimental analysis and observation.

Results of recent synchrotron XPS/EXAFS studies of pure and supported clusters and colloids reveal their unique electronic properties and highlight the importance of support chemistry in controlling aggregation of clusters.3, 4 We applied density functional theory to model a wide range of clusters in order to assign core and core-ligand vibrations in experimentally obtained spectra for the first time.5,6

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Keywords

atomically precise clusters, unique electronic properties, DFT calculations predicting experiment

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