



### STABILITY AND MECHANICAL PROPERTIES OF HIGH-COORDINATED GROUP IV METAL DIOXIDES

Dr. Varghese Swamy

ARC Centre of Excellence for Design in Light Metals, Department of Materials Engineering  
Monash University

**Tuesday 24<sup>th</sup> June 2008, 4:00 p.m. – 5:00 p.m.**  
**Science Lecture Theatre S10**

High-coordinated Ti, Zr, and Hf dioxides have received significant attention as potential ultrastiff/ultrahard substances. Cotunnite-TiO<sub>2</sub> (OII) with nine-fold metal-oxygen coordination synthesized at ~60 GPa represents the stiffest and hardest of the oxides identified to date. Other proposed high-density structures (stable at high-pressures) include an orthorhombic phase (OI), a pyrite-structured phase, and a fluorite-structured phase. Good agreements have been obtained between experimental and *ab initio* results on the elastic properties of most of the phases; however, a major discrepancy has emerged between the available experimental and theoretical elastic data on pure and Zr-substituted cubic TiO<sub>2</sub>. This presentation will discuss the results of our first-principles calculations with a focus on the elastic properties of the cubic phases. A detailed comparison of the effects of the functionals used (density-functional and hybrid density-functional –Hartree-Fock approaches) on the computed elastic properties and ground state as well as that between the theoretical and experimental data will be presented.

Varghese Swamy has been working as a Senior Research Fellow at Monash University (in the Department of Materials Engineering and at the ARC Centre of Excellence for Design in Light Metals) since 2003.

Visitors are most welcome: Please note the parking arrangements. There is a designated Visitors Car Park (N1) clearly ground-marked by white paint and tickets, at a cost of \$3/day, are available from a dispensing machine. ('Blue' permit designated areas are for Monash members only.). It is also possible to park at other designated Visitors Car Parks (E1, S1 and S2) on the Clayton Campus, but tickets are \$1.4/hour.

Convenor: Dr. Jian-Feng Nie  
Tel: 9905 9605  
Email: [nie@eng.monash.edu.au](mailto:nie@eng.monash.edu.au)