ICAMS

INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

Special Seminar

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Tuesday, September 21, 1:30 p.m.
ICAMS seminar room UHW 11/1102

Interatomic forces in oxides

Several approaches to the atomistic simulation of oxides have been used over the last fifty years, ranging from simple ionic models (Born), electron-gas models (Gordon-Kim), shell models (Overhauser), Charge transfer models (Streitz-Mintmire), multibody interactions (Wilson-Madden, Scandalo-Tangney), tight-binding and others. I will review the relationship between these approaches and some of their successes and failures compared to first-principles calculations, with particular reference to my own group's experience with ZrO_2, Al_2O_3 and $SrTiO_3$ and defect chemistry.