INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

**ICAMS Special Seminar**

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Room IC 02-722

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## First-principles calculation of oxygen self-diffusivity in zirconia

A first-principles calculation of the self-diffusivity of oxygen in tetragonal $ZrO_2$ has been attempted based on the atomistic theory of diffusion using the electronic structures, phonon vibration spectrum combing the transition state theory (TST). A local harmonic approximation (LHA) that captures the most important vibrations adjacent to the migrating atom is proposed in the present work to deal with the dynamic instability of tetragonal $ZrO^2$ which is stable above 1478K, the absolute values of correlation factors, atom jump frequencies along a-axis and c-axis directions for a tetragonal lattice have been evaluated respectively. Together with the calculated vacancy concentration, the oxygen self-diffusion coefficients along a-axis and c-axis as the functions of temperature and oxygen partial pressure are obtained for tetragonal $ZrO_2$, which shows that the calculated values with a partial oxygen pressure of 10-15 atm compares well with the available experimental measurements in $ZrO_2$.