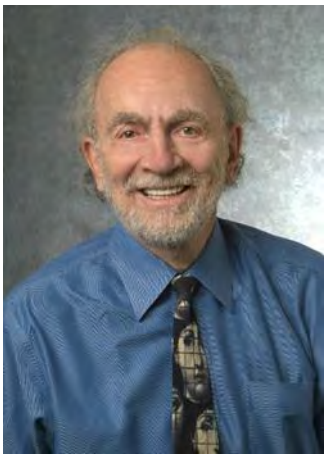
東京大学
微細構造解析
プラットフォーム
The University of Tokyo

東京大学微細構造解析プラットフォーム
公開講演会

“The Semiconductor Physics of Sapphire (α-Al2O3): Defect Chemistry and the Fermi Level”



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Abstract

Point defect energetics of pristine α-Al_2O_3, and α-Al_2O_3 doped with the aliovalent solutes MgO and TiO_2, have been calculated as a function of the Fermi level using DFT, employing the hybrid HSE potential. Migration barriers have also been calculated for oxygen and Al vacancies and oxygen and Al interstitials. Surprisingly, the calculations for pristine Al_2O_3 are consistent with lattice diffusion data for oxygen and Al. This suggests, contrary to expectations, that the expected variation of lattice diffusivities with impurity content has been “buffered,” a phenomenon that has come to be known as the “corundum conundrum.” The buffering mechanism is still not known with certainty.

September 12 (Fri), 2014 15:00～16:30
Main meeting room at Institute of Engineering Innovation, UT
(工学部総合研究機構　9 号館 1 階　大会議室)
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