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Point defects and diffusion in Al_2 O_3 NICHOLAS HINE, KILIAN FRENSCH, MATTHEW FOULKES, MIKE FINNIS, Imperial College London, ARTHUR HEUER, Case Western Reserve University — Reconciling experimental measurements of self-diffusion in Al_2O_3 with theoretical calculations has long been problematic. Measured activation energies and diffusion coefficients are inconsistent with calculations, and the effect of aliovalent impurity doping is much smaller than is usual in such materials. We report *ab initio* calculations using DFT and DFPT of temperature-dependent formation energies and migration barriers of a wide range of native point defects and defect-impurity clusters, parameterized by the constituent species chemical potentials. Using these energies as inputs to a mass-action analysis, we predict how defect concentrations depend on temperature, oxygen partial pressure and impurity doping. Finally, the formation energies are combined with migration barriers to provide diffusion activation energies, and thus an explanation of self-diffusion in alumina. We are able to account in a consistent way for experimental results and resolve the long-standing "corundum conundrum." The importance of determining the Fermi energy self-consistently within a mass-action framework is demonstrated, and the surprising insensitivity of the diffusion coefficients to aliovalent impurity doping is shown to result from a "buffering" mechanism relating to clustering of defects and dopants that should also occur in other ionic materials.

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