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First-Principles Modeling of ThO_2 Solid Solutions with Oxides of Trivalent Cations VITALY ALEXANDROV, Department of Chemical Engineering and Materials Science, and NEAT Organized Research Unit, University of California, Davis, MARK ASTA, Department of Chemical Engineering and Materials Science, University of California, Davis, NIELS GRONBECH-JENSEN, Department of Applied Science, University of California, Davis — Solid solutions formed by doping ThO_2 with oxides of trivalent cations, such as Y_2O_3 and La_2O_3, are suitable for solid electrolyte applications, similar to doped zirconia and ceria. ThO_2 has also been gaining much attention as an alternative to UO_2 in nuclear energy applications, the aforementioned trivalent cations being important fission products. In both cases the mixing energetics and short-range ordering/clustering are key to understanding structural and transport properties. Using first-principles atomistic calculations, we address intra- and intersublattice interactions for both cation and anion sublattices in ThO_2-based fluorite-type solid solutions and compare the results with similar modeling studies for related trivalent-doped zirconia systems.

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