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First-principles study of Oxygen vacancies in $Mg_xZn_{1-x}O$ alloys
ADISAK BOONCHUN, WALTER LAMBRECHT, Case Western Reserve University — A first principles study of oxygen vacancies in $Mg_xZn_{1-x}O$ alloys has been carried out within the LDA+$U_s + U_d$ FP-LMTO approach. Different types of oxygen vacancies are distinguished by their number of Mg and Zn nearest neighbors. We find that the energy of formation is lowest for oxygen vacancies surrounded by four Zn nearest neighbors. Because of the Boltzmann factor this implies that the probability of finding oxygen vacancies with one or more Mg as nearest neighbors is strongly suppressed. Unlike in pure ZnO and MgO, we do not find negative U behavior but this may in part be because of the small size of the supercell. The 2+/+ and +/0 transitions level gradually move to higher energy as the number of nearest neighbor Mg atoms increases. Defect levels in rocksalt MgO are also presented.

Adisak Boonchun
Case Western Reserve University

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