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Ab initio investigations of complex oxides ALTYNBEK MURAT, JULIA E. MEDVEDEVA, Missouri University of Science & Technology — We employ *ab-initio* density functional approach to investigate the structural, optical and electronic properties of twelve complex oxides with layered structure $RAMO_4$, R=In or Sc, A=Al, Ga, M=Ca, Cd, Mg, and/or Zn. We find that presence of the light metal (e.g., Al, Ca, Mg and Sc) oxides significantly affects the optical band gap which varies from 0.64 eV ($InGaCdO_4$) to 4.35 eV ($ScAlMgO_4$). At the same time, the electron effective mass remains nearly isotropic in all oxides, and both structurally and chemically distinct layers are expected to participate in charge transport once the materials are degenerately doped. Further, for a comparative systematic investigation of carrier generation mechanisms in complex oxides, we calculated the electronic properties of fluorine doped (F_O) and oxygen-reduced $RAMO_4$ materials as well as their single-cation constituents in various phases. We determine most preferable spatial distribution of the F impurity and the oxygen defect in the layered structure of each material and find that the dopant/vacancy site locations correlate with the formation energy of the single-cation oxides. The results allow us to draw conclusions on the role played by each constituent oxide and to predict how the properties of multicomponent materials can be controlled via chemical composition, crystal structure and carrier generation.

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