Ab-Initio Study of Defect Physics for Layered LaCuChO and BaCuChF (Ch={S,Se,Te}) Structures

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genides LnCuChO (Ln = {La,Pr,Nd}, Ch = {S,Se,Te}) and isostructural layered flu-
orochalcogenides BaCuChF have drawn much interest in recent years as p-type wide
bandgap semiconductors with applications in transparent electronics and photo-
voltaics. Previous experimental and computational studies concluded for both LaCu-
ChO, with a bandgaps between 2.4-3.1 eV, and BaCuChF, with optical bandgaps
between 2.8-3.5 eV, that p-type conductivity is primarily due to copper vacancies.
We report a comparative ab-initio computational study of the defect physics for both
families of materials. Point defects and defect complexes are taken into account and
previously omitted corrections have been included.\textsuperscript{1,2} Accurate chemical potential
stability diagrams and formation energies are calculated using the GGA+U method
and fitted elemental-phase reference energies.\textsuperscript{3}

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Date submitted: 17 Dec 2012

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