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Ab initio study of $Ba_{1-x}Sr_xSnO_3$ and $BaSn_{1-x}M_xO_3$ (M = Bi, Pb) using the ACBN0 functional: structural, electronic and optical properties HAIHANG WANG, University of North Texas, PRIYA GOPAL, MARCO FORNARI, Central Michigan University, STEFANO CURTAROLO, Duke University, ICHIRO TAKEUCHI, University of Maryland, MARCO BUONGIORNO NARDELLI, University of North Texas — Using the recently developed pseudohybrid Hubbard density functional ACBN0 [1], we have studied the structural, electronic and optical properties of $Ba_{1-x}Sr_xSnO_3$ and $BaSn_{1-x}M_xO_3$(M = Bi, Pb). This study is motivated by recent experimental results which show that the solid solutions of $BaSnO_3$ mixed with Bi, Sr or Pb remain transparent for a wide range of mixing ratio (up to 40 percent). While traditional DFT calculations on native $BaSnO_3$ and $BaBiO_3$ fail to open the gap (both systems result as semi-metals), thereby hindering the study of related materials, we demonstrate that using ACBN0, the band gaps open and are in good agreement with experiments. Particularly, in $BaBiO_3$, we correctly reproduce the crystal structure instability caused by the well-known breathing and tilting modes of the oxygens, and the alternating ordering of Bi^{3+} and Bi^{5+} ions. A detailed theoretical investigation of the alloyed systems together with some most recent experimental results will be discussed. [1] L.A. Agapito, S. Curtarolo, and M. Buongiorno Nardelli. *Reformulation of DFT+U as a Pseudohybrid Hubbard Density Functional for Accelerated Materials Discovery,* Phys. Rev. X **5,** 011006 (2015).

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