Topological Transition in Pb$_{1-x}$Sn$_x$Se
Using Meta-GGA Exchange-Correlation Functional


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We calculate the mirror Chern number (MCN) and the band gap for the Pb$_{1-x}$Sn$_x$Se alloy as a function of the concentration $x$ by using a virtual crystalline approximation. We use the electronic structure from the relativistic density functional theory calculations in the Generalized-Gradient-Approximation (GGA) and meta-GGA approximation. Our results obtained with the modified Becke–Johnson meta-GGA functional are comparable with the available experimental data for the MCN as well as for the band gap. We advise to use the modified Becke–Johnson approximation with the parameter $c = 1.10$ to describe the transition from a trivial to topological phase for this class of compounds.

This article was originally published in October 2019 with erroneously swapped captions of Figs. 1–5. The captions of Figs. 1–5 should be corrected in the following way:

- Fig. 1 should have the caption of Fig. 5,
- Fig. 2 should have the caption of Fig. 1,
- Fig. 3 should have the caption of Fig. 2,
- Fig. 4 should have the caption of Fig. 3,
- Fig. 5 should have the caption of Fig. 4.

The Editors apologize for this error.