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Ga acceptors in SnO_2 revisited: A hybrid functional study

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SnO_2 is an oxide semiconductor with wide band gap, good transparency, and high thermal and chemical resistances. As-grown SnO_2 usually exhibits *n*-type conductivity with high carrier concentrations, which is an obstacle to make it *p*-type. Consequently, applications of SnO_2 for optoelectronics are limited. Group-III elements, such as Al, Ga, and In, are candidates to give *p*-type conductivity when substituting for Sn in SnO_2. Earlier calculations suggested that the calculated results of these dopants can be shallow or deep depending on the computational details, i.e., the result based on HSE calculations [Phys. Rev. B **79**, 245206 (2009)] showed that they are shallow acceptors, on the other hand, PBE0 calculations [J. Mater. Chem. **22**, 25236 (2012)] showed that they are all deep. In this work, the possibility of making *p*-type SnO_2 by Ga was revisited using the HSE functional. Our results show that the acceptor level of Ga_{Sn} is actually deep. Therefore, Ga can only serve as compensating acceptor but not a *p*-type dopant for SnO_2. This conclusion does not change even after the alloying of SnO_2 with Si ($Si_xSn_{1-x}O_2$ where $x \sim 0.17$) to introduce a compressive strain.

Summary

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