Chemical doping of nano-structured PbS

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Galium oxide family are wide-gap semiconductors, and their optical features, tunable by impurity dope, are expected to be useful for many applications. In order to analyze our experimental data of photo-absorption/luminescence affected by the impurities in Ga_2O_3 [1], electronic states of ϵ- and κ-Ga_2O_3 with Co dope were calculated using the VASP code [2] based on first principles theory.

Calculations were done for a single unit cell through supercells sized to 8×4×4, with/without Co dope as an impurity atom. The calculation was typically done in one or four computer-nodes, in *hybrid* parallelism (8 MPI × 3 openMP par node, typically). We began with the optimization without the impurity. The lattice constants were fixed at the obtained optimized dimension, and a Ga atom was then replaced by Ge. As expected from the small lattice constant of **b** and **c** direction, 1×1×2 or 1×2×1 supercell of Ga_2O_3 gave instable results, suggesting necessity of careful conformation of the impurity to avoid the Co-Co interaction at high density of the impurity.

The results in density functional theory (DFT) gave Co-induced states in the band gap (see the main panel of Figure 1). They are not satisfactory in that the calculated band gap did not agree with the experimental data, as often seen in DFT. Thus we concluded some modification should be introduced, such as empirical methods namely DFT+U or non-local external potential (NLEP) [3]. However, the tendency of bandgap increase/decrease in the calculated results (inset of Fig.1) was in good agreement with out experimental results.

At the same time, we performed preliminary calculation of impurity states in PbS crystal, and detailed analysis of spin-polarization of monolayer film of metal organic framework (MOF) started as an ISSP project (H29-Cb-0009) from 2018.

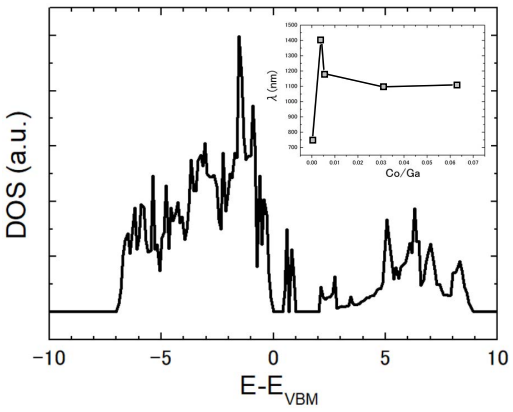

Figure 1: Calculated density of electronic states with a Co atoms in a 8×4×4 ϵ-Ga_2O_3 supercell. Inset: band-gap to varied density of the Co impurity.

References

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[3] S. Lany, H. Raebiger, and A. Zunger: Phys. Rev. B 77, 241201 (2008).