First-principles calculations of Berry curvature: WTe2 and other heavy metals

Sung-Hyon Rhim*
Department of Physics and Energy Harvest Storage Research Center, University of Ulsan, Republic of Korea
sonny@ulsan.ac.kr

With rapid progress in spintronics, utilizing the spin Hall effect (SHE) or the interface spin phenomena has become highly demanding for practical applications with high interests. In this sense, calculation of spin Hall angle (θ_{SH}) or Berry curvature (Ω_z) based on first-principles calculations is of great significance in exploration for materials. Here, we adapt the method proposed by previous work, which has been implemented in FLAPW method. As large spin Hall angle has been reported in tungsten, calculations on tungsten metals - for bcc and A15 structure are presented. Also results on WTe2 are shown further, where the nonsymmorphic feature of space group plays some important role. Results of other heavy metals are also reviewed for reference.

References

[1] G. Y. Guo, S. Murakami, T.-W. Chen, and N. Nagaosa, Phys. Rev. Lett. **100**, 096401 (2008).
[2] Kai-Uwe Demasius and et al. Nat. Comm. **7**, 10644 (2016).