Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-principles calculations of Berry curvature for Tungsten metals and compound[1] SONNY H. RHIM[2], University of Ulsan — With rapid progress in spintronics, utilizing spin Hall effect or 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 significant in exploration for materials search. Here, we adapt the method proposed by previous work [3], which has been implemented in FLAPW method. As large spin Hall angle has been reported in tungsten [4], calculations on tungsten metals - for *bcc* and $A15$ structure are presented. Also results on WTe_2 are shown further.

[1]This research was supported by Creative Materials Discovery Program through the National Research Foundation of Korea (2015M3D1A1070465).
[2]U. Wisconsin-Milwaukee
[3]G. Y. Guo, S. Murakami, T.-W. Chen, and N. Nagaosa, Phys. Rev. Lett. **100**, 096401 (2008).
[4]Kai-Uwe Demasius and *et al.* Nat. Comm. **7**, 10644 (2016).

Sonny H. Rhim
University of Ulsan

Date submitted: 11 Nov 2016 Electronic form version 1.4