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Berry Phase and *Ab initio* Calculation of Anomalous & Spin Hall Effect

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Berry phase in momentum space in spin-orbit coupled bands affects the charge and spin transport of electrons in real space, and produces fascinating new phenomena. Two examples are the anomalous Hall effect and the recently proposed intrinsic spin Hall effect. Avoiding the ambiguity introduced by model Hamiltonians, we evaluate the Berry curvature accurately for real materials by parameter-free *ab initio* methods. We have calculated the anomalous Hall conductivity for ferromagnetic crystals of Fe, Co, Ni, Mn_5Ge_3, and $CuCr_2Se_{4-x}Br_x$, and investigated the magnetization dependence and sign change, with results in quantitative agreement with experiments [1,2]. Using the *ab initio* technique, we have also evaluated the intrinsic spin Hall conductivity in non-magnetic semiconductors (GaAs, Si, Ge, AlAs) as well as metals (W and Cu) [3,4]. We have systematically studied how its sign and magnitude depend on strain, doping density, and frequency for the semiconductors, and found very large values for the metals. [1] Yugui Yao *et al.*, *Phys. Rev. Lett.* 92, 037204 (2004). [2] Changgan Zeng, Yugui Yao, Qian Niu, and Hanno, H. Weitering, (*Phys. Rev. Lett.* in review). [3] Yugui Yao and Zhong Fang, *Phys. Rev. Lett.* 95, 156601 (2005). [4] Guangyu Guo, Yugui Yao, Qian Niu, *Phys. Rev. Lett.* 94, 226601 (2005).