Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Intrinsic circular polarization in centrosymmetric stacks of transition-metal dichalcogenide[1] QIHANG LIU, XIUWEN ZHANG, ALEX ZUNGER, University of Colorado, Boulder — The circular polarization (CP) that the photoluminescence inherits from the excitation source in n monolayers of transition-metal dichalcogenides $(MX_2)_n$ has been previously explained as a special feature of odd values of n, where the inversion symmetry is absent. This valley polarization effect results from the fact that in the absence of inversion, charge carriers in different band valleys could be selectively excited by different circular polarized light. Such restriction to non-centrosymmetric systems poses a limitation on the material selection for achieving CP. Although several experiments observed CP in centrosymmetric MX_2 systems e.g., for bilayer in MX_2, they were dismissed as being due to some extrinsic sample irregularities. Here we show that also for n = even where inversion symmetry is present and valley polarization physics is strictly absent, such intrinsic selectivity in CP is to be expected on the basis of fundamental spin-orbit physics. First-principles calculations of CP predict significant polarization for n = 2 bilayers: from 69% in MoS_2 to 93% in WS_2. This realization could broaden the range of materials to be considered as CP sources.

[1]This work was supported by National Science Foundation (Grant No. DMREF-13-34170).

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Date submitted: 13 Nov 2014 Electronic form version 1.4