Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Nonequilibrium spin texture within a thin layer below the surface of current-carrying topological insulator Bi2Se3: A first-principles quantum transport study[1] PO-HAO CHANG, BRANISLAV NIKOLIC, Univ of Delaware, TROELS MARKUSSEN, SREN SMIDSTRUP, KURT STOKBRO, QuantumWise — Using extension of nonequilibrium Green function combined with density functional theory (NEGF+DFT) formalism to situations involving noncollinear spins and spin-orbit coupling, we investigate microscopic details (on the 1 A scale) of nonequilibrium spin density S(r) driven by unpolarized charge current injection into a ballistic thin film of Bi 2 Se 3 as prototypical topological insulator (TI) material. We find large nonzero component of S(r) in the direction transverse to current flow on the metallic surfaces of TI, as well as within few bulk atomic layers near the surfaces because of penetration of evanescent wavefunctions from the metallic surfaces into the bulk. In addition, an order of magnitude smaller components emerge in the perpendicular (within surfaces and nearly bulk regions of TI) and longitudinal (within bulk region of TI near its surface) directions, thereby creating a complex nonequilibrium spin texture. We also demonstrate how DFT calculations with properly optimized local orbital basis set can precisely match putatively more accurate calculations with plane wave basis set for the supercell of Bi 2 Se 3 .

[1]P.-H.C. and B.K.N. were supported by NSF Grant No. 281 FQ ECCS 1509094. The supercomputing time was provided by 282 XSEDE, which is supported by NSF Grant No. ACI-1053575. 283 QuantumWise acknowledges support from the Danish Inno- 284 vation Fund Grant No

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Date submitted: 06 Nov 2015 Electronic form version 1.4