Abstract Submitted
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Theoretical study on quantum spin Hall phases in bismuth ultrathin films SHUICHI MURAKAMI, Tokyo Institute of Technology and PRESTO, JST, MASAKI WADA, Tokyo Institute of Technology, FRANK FREIMUTH, GUSTAV BIHLMAYER, Forschungszentrum Juelich — It has been proposed that the (111) 1-bilayer bismuth is in the quantum spin Hall phase [1]. This argument is based on a simple tight-binding model for the 3D bismuth, and it is desirable to examine this result by more realistic methods. In this presentation, we investigate possibilities of the quantum spin Hall phases in two of the bismuth ultrathin films by first- principle calculations and confirmed the result in Ref.[1]. Bulk bismuth is a semimetal, while some of the bismuth ultrathin films have a gap. As proposed by first-principle calculations, among various phases seen in experiments, only two cases are gapped: (i) (111) 1-bilayer film and (ii) {012} 2-monolayer film. These two structures are almost degenerate in energy. We calculate the Z_2 topological numbers for the two structures. both from the bulk Bloch wavefunctions and from band structure calculations in the geometry with edges. In the calculations we use the maximally localized Wannier orbitals constructed from first-principle calculations. We found that (i) is the quantum spin Hall phase while (ii) is an ordinary insulator. Their difference can be observed in STM/STS and other possible experiments to verify our results are discussed. [1] S. Murakami, Phys. Rev. Lett. 97, 236805 (2006).

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