Orbital magnetization of quantum spin Hall insulator nanoparticles

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Supporting Information

The edge type and nanoisland shape dependence

We have verified that the orbital magnetization occurs regardless of the edge type and nanoisland shape. In Fig. S1 we show an evolution of energy spectra in a magnetic field of **a** triangular nanoisland with zigzag edges, **b** hexagonal nanoisland with armchair edges, **c** hexagonal nanoisland with structural edge disorder. All these spectra are calculated using the same four-orbital tight-binding model discussed in the text.[1] Whereas the distribution of level spacings δ of the islands with armchair edge and the one with a disordered edge is less regular than in the case of islands with ideal zigzag edges, all of them show a strong orbital magnetization, as reflected by the large splitting induced by a magnetic field. Results presented in Fig. S1 are in agreement with an analysis from Ref.[2] regarding an existence of

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topologically protected edge states for structures with arbitrary edge orientation. For the island with dangling atoms a linear splitting in a magnetic field for many in-gap states is still observed. These calculations confirm the presence of orbital magnetization in arbitrary shape and type of edges QSHI nanoislands.

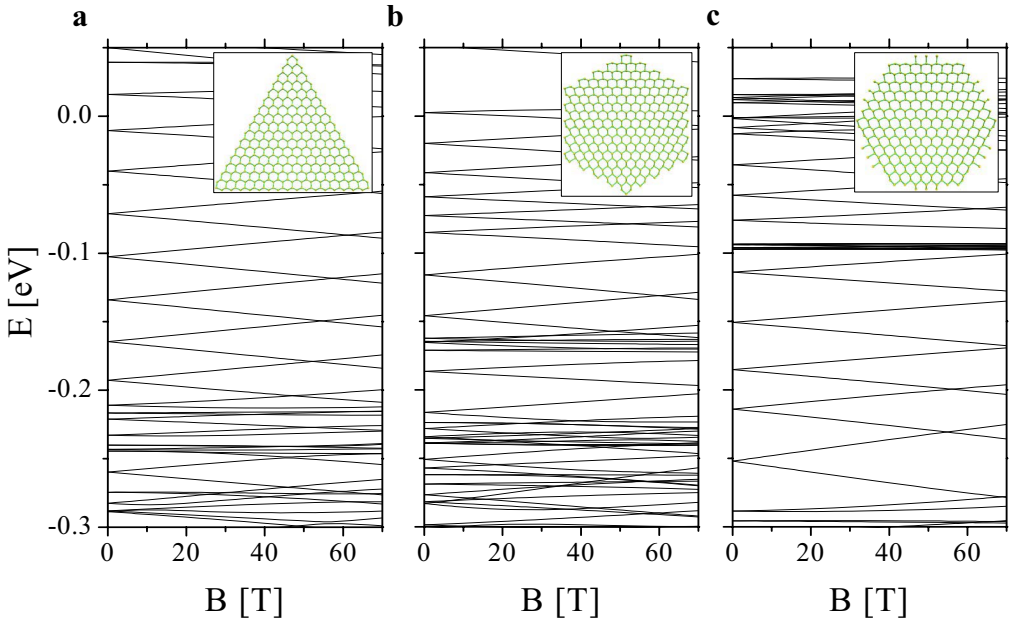

Figure S1: **Shape effect.** An evolution of energy spectra in a magnetic field of **a** triangular nanoisland with zigzag edges, **b** hexagonal nanoisland with armchair edges, and **c** hexagonal nanoisland with structural edge disorder. For all structures some set of states reveal linear splitting in a magnetic field.

Influence of the substrate

We now address the influence of the interaction with the substrate on the orbital magnetization. Motivated by the experiments by Drozdov and coworkers,[3] where the Bi(111) flakes were located on the surface of a thin film of Bi(111), we compute the spectrum for an hexagonal nanoisland such as the one in the main text, with $L \simeq 3.6$nm ($N = 384$ atoms), on top of a much larger Bi(111) island with dimensions 50×55nm ($N = 31240$ atoms). Periodic boundary conditions are assumed along one direction (see Fig. S2**a**) so that the substrate edges are disconnected. Full diagonalization of Hamiltonian matrix of such a big system (in

this case size of Hilbert space $\sim 3*10^5$) is not possible, so we find only a set of eigenstates in a vicinity of bilayer energy gap E_{gap} using iterative eigensolver method.[4] The energy splittings for $B = 1T$, both with (inset) and without (main panel) coupling to the substrate, are shown in Fig. S2**b**. We focus on the energy range given by the in-gap region, taking the gap E_{gap}, from the two dimensional Bi (111) bilayer, which is marked by vertical red dash lines. We find additional in-gap states of the supported island, compared to the freestanding one, that correspond to substrate edge states, as inferred from inspection of their wave functions. In the inset we assign a color code to the states: red stands for substrate states, blue for island states. Whereas the evolution of the magnetic moments as a function of energy is no longer a smooth function, it is still apparent that many in-gap states retain their orbital magnetization. The substrate in-gap states have a very small splitting (red points). Thus, our calculations suggest that orbital edge currents could still be present in Bi(111) flakes deposited on Bi(111). We have also verified that similar results hold for larger islands, with $L \simeq 9$ nm edge length ($N = 2400$ atoms) deposited on the same substrate.

A magnetic field dependence

A magnitude of maximum orbital moment as a function of applied magnetic field is investigated in Fig. S3. The inset shows a corresponding energy levels evolution in a magnetic field (a green line indicates a state generating M_{max}). The magnetic moment is stable, only slightly decreasing, up to $B = 70$T. When a crossing of a given state with other state occurs, e.g. for $B = 40$T, see the inset, there is no change of orbital moment due to no change of a slope of energy level in B. On the other hand, when two states anticross, e.g. for $B = 80$T, it results in a drop of the orbital moment. When anticrossing region is left, magnetic moment return to its high value.

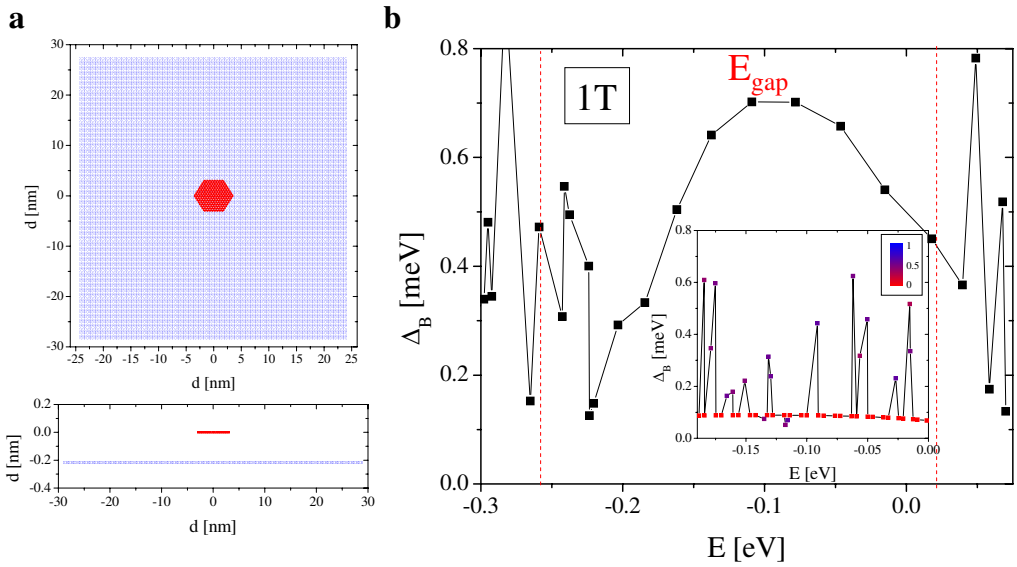

Figure S2: **Interaction with substrate. a** Nanoisland with $L \simeq 3.6$nm ($N = 384$ atoms) deposited on 50×55nm ($N = 31240$ atoms) substrate from top(upper panel) and side(lower panel) view. In order to reduce edge effects from the substrate, periodic boundary conditions in one direction were applied. Energy splitting of Kramer's degenerate pairs ΔE_B for a magnetic field $B = 1$T without the substrate is shown in a main panel and with the substrate in the inset. The Bi (111) bilayer energy gap E_{gap} is indicated by red dash lines. The states localized within nanoisland are found by calculating electronic probability densities for each energy eigenstate. States fully localized in the substrate are indicated by red color while states fully localized in nanoisland by blue color.

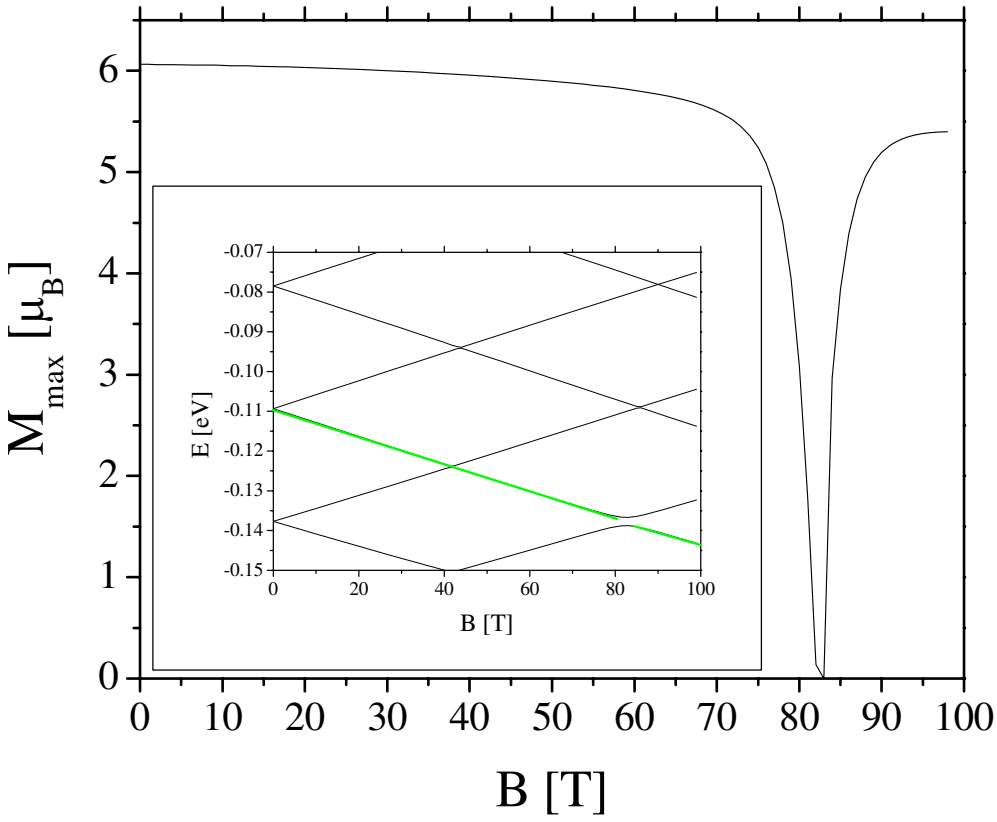

Figure S3: **Magnetic field dependence. a** Maximum orbital moment M_{max} as a function of applied magnetic field for nanoisland with $L \simeq 3.6$nm ($N = 384$ atoms). The inset shows an evolution of energy levels as a function of a magnetic field. A green line indicates an energy level generating M_{max}.

Orbital nanomagnets with other Hamiltonians

In order to check universality of orbital nanomagnetism in QSHI nanoislands, we model them with the Kane-Mele Hamiltonian.[5] This model, widely used to describe the QSH phase, is a good approximation for materials such as graphene and Silicene.[6] It features a single orbital per atom and the spin-orbit interaction is given by a spin-dependent second neighbor hopping. In the presence of an external magnetic field the Hamiltonian is written as

$$H_{KM} = t \sum_{\langle i,j\rangle,\sigma} e^{i\phi_{ij}} a^{\dagger}_{i\sigma} a_{j\sigma} + i\lambda_{SO} \sum_{\langle\langle i,j\rangle\rangle\alpha\beta} v_{ij} s^{z}_{\alpha\beta} a^{\dagger}_{i\alpha} a_{j\beta}, \tag{1}$$

with summation in the first term over nearest neighbors and in the second term over next nearest neighbors, and $v_{ij} = \pm 1$ for clockwise and counterclockwise direction of path connecting site i and j, s^z is a Pauli matrix and λ_{SO} strength of effective spin-orbit coupling. We have simulated a hexagonal nanoisland with armchair edges consisting of $N = 1986$ atomic sites and $L = 4.4$nm. In Fig. S4 the evolution of the energy spectrum as a function of magnetic field is shown. Again, our calculations yield a linear splitting of Kramers doublets with a magnetic field around energy $E = 0$. Using the same argumentation of the main text, this should lead to the generation of persistent edge currents whenever a single electron occupies the highest occupied Kramers doublet. In the inset, we show the size-scaling of maximal magnetic moment M_{max} from these states, and we find a linear scaling, consistent with the behavior expected for Dirac electrons in a ring.

Finally, we note that quantum dots described with the Hamiltonian proposed by Bernevig-Hughes-Zhang (BHZ) to predict the QSHI phase CdTe/HgTe quantum wells,[7] as well as in III-V type II structures,[8] also lead to the existence of in-gap edge states[9] in the dots endowed with orbital magnetization. Therefore, the concept of orbital nanomagnet built with zero dimensional nanostructures of quantum Hall insulators is a model-independent prediction.

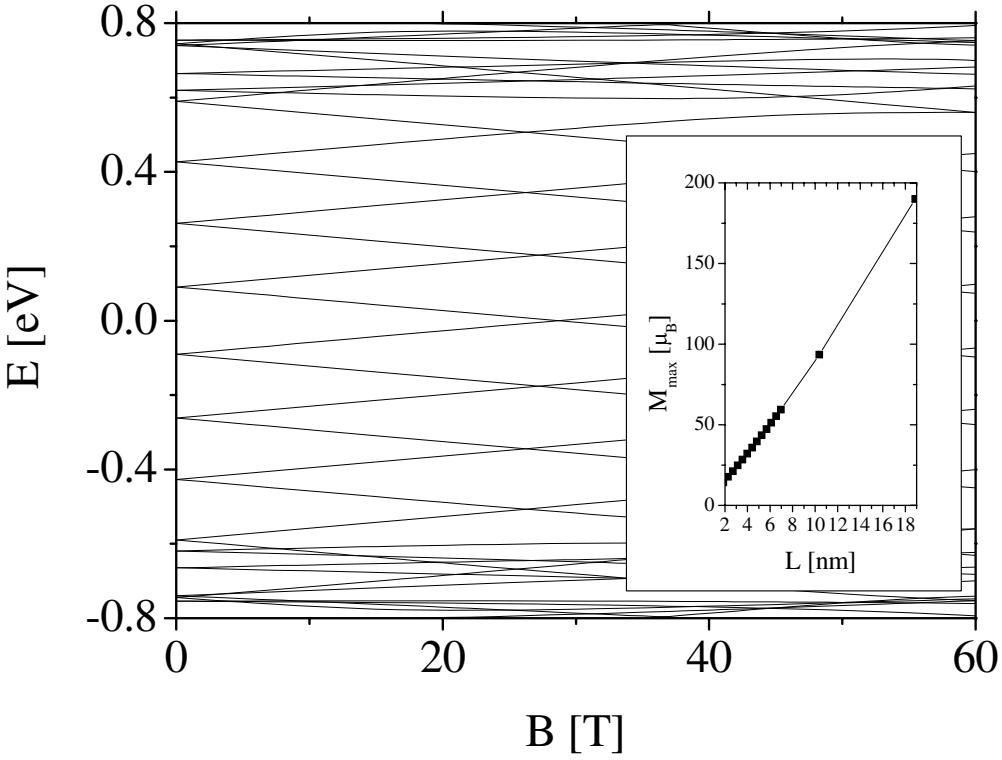

Figure S4: **Nanoisland within Kane-Mele model.** An evolution of energy spectra in a magnetic field of hexagonal nanoisland with armchair edges with $N = 1986$ atoms and $L = 4.4$nm calculated within Kane-Mele model for $t = -3.0$eV and $\lambda_{SO} = 10$meV. In a vicinity of the middle of the energy spectrum, $E = 0$ a set of linearly dispersed states in a magnetic field is clearly seen. The inset shows a linear dependence of maximal orbital magnetic moment M_{max} as a function of nanoisland edge length L.

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