Revealing the topological phase diagram of $ZrTe_5$ using the complex strain fields of microbubbles

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Abstract

Topological materials host robust properties, unaffected by microscopic perturbations, owing to the global geometric properties of the bulk electron system. Materials in which the topological invariant can be changed by easily tuning external parameters are especially sought after. Zirconium pentatelluride ($ZrTe_5$) is one of a few experimentally available materials that reside close to the boundary of a topological phase transition, allowing the switching of its invariant by mechanical strain. We unambiguously identified a topological insulator - metal transition as a function of strain, by a combination of *ab initio* calculations and direct measurements of the local charge density. Our model quantitatively describes the response to complex strain patterns found in bubbles of few layer $ZrTe_5$ without fitting parameters, reproducing the direction dependent closing of the band gap observed using scanning tunnelling microscopy. We calculated the topological phase diagram of $ZrTe_5$ and identify the phase at equilibrium, enabling the design of device architectures which exploit the unique topological switching behaviour.

Figures

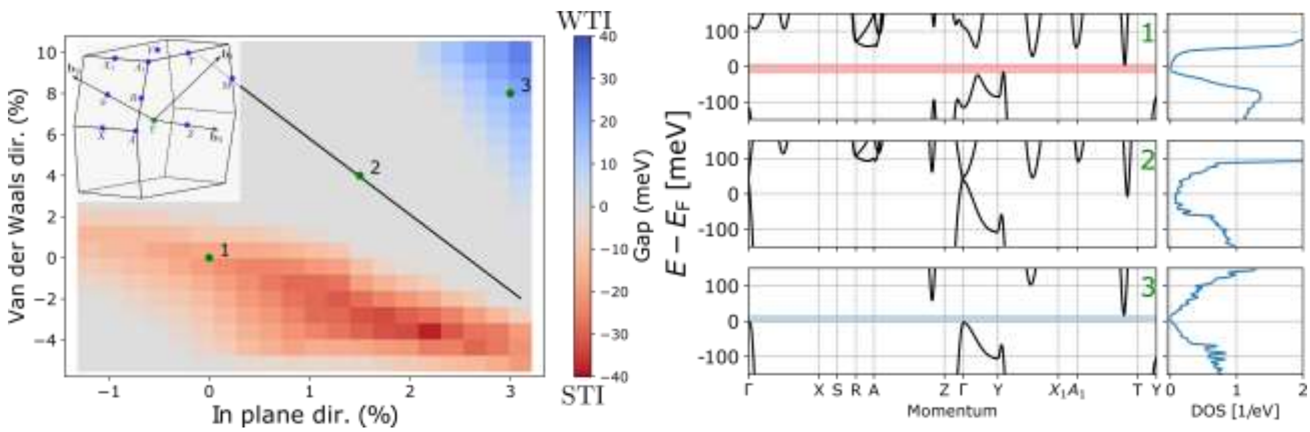

Figure 1: Left: The phase diagram of the electronic structure of the crystal under mechanical strain. At every point the size of the gap was calculated (SIESTA) and a sign has been assigned to it according to the topological flavour of the gap. The negative gap corresponds to the strong topological insulating phase, while the positive gap to the weak topological phase. The green dots assigned with a number denote the corresponding band structure on the right panel. The inset shows the corresponding Brillouin zone indicating the high symmetry points. Right: The calculated band structure along the path of the high symmetry points. The opaque band shows the size of the gap and colour indicates the topological favour.