Electronic and topological properties of Twisted Plumbene

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Since the discovery of graphene in 2004, researchers have been studying two-dimensional materials including the group IV family of the periodic table, such as graphene, silicene, germanene, stanene, and plumbene [1]. In 2005, Kane and Mele proposed $\mathbb{Z}_2$ topological order in a study of spin-orbit interactions on the electronic structure of graphene. However, the weak spin-orbit coupling in graphene only allows for topological properties to appear at extremely low temperatures due to the tiny electronic band gap at the Dirac point [2]. In the $\mathbb{Z}_2$ topological insulator, the edges of the material are conducting while the bulk of the material is an insulator.

The SOC interaction opens an electronic band gap energy in the hexagonal lattice of group IV elements. But the topologically protected gap is not sufficient for operation at room temperature [3, 4, 5]. The last member of this group, plumbene the atomic Pb monolayer in group IV with a similar structure and large band gap opening at room temperature which the synthesis recently [6, 7]. The calculation of the $\mathbb{Z}_2$ topological invariant shows that plumbene is a topologically trivial insulator [8]. The number and arrangement of layers, the types of layers added on top of each other, and the rotation angle of the layers to each other can affect the electronic and topological characteristics of van der Waals. It was shown that if thin layers are separated from a van der Waals crystal and reconnected at a specific angle, the resulting structure will display a planar Moiré pattern with a larger periodicity than the original structure, leading to different characteristics. The recent discovery of the magic-angle bilayer graphene (1.1 degrees) that makes a phase transition to superconductor has led to the rapid growth of twistronics, a new field in condensed matter physics [9, 10].

In the present study, analyzing the dependence of electronic and topological properties on the twisting angle in twisted bilayer plumbene structures has been performed within the framework of Density Functional Theory (DFT) as implemented in the OpenMX computational package. We calculated the $\mathbb{Z}_2$ topological invariant by the Fukui-Hatsugai method which is based on lattice Chern numbers [11, 12]. We examine the electronic band structures at various twisting angles from 0 to 60 degrees. Our results indicate the potential for a trivial to topological insulator phase transition in plumbene at specific angles.

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