Localized Spin-orbit Polaron in Magnetic Weyl Semimetal $Co_3Sn_2S_2$

The defect engineering of magnetic quantum materials and the regulation of local spins are expected to play a key role in building practical quantum spin devices in the future, which is currently one of the hotspots in condensed matter physics research. The transition-metal-based kagome lattice compounds have merged recently as a novel materials platform for unveiling and exploring the rich and unusual physics of geometric frustration, correlation and magnetism, and the topological behaviors of the quantum electronic states. These are layered crystalline materials where the transition metal elements occupy the vertices of the two-dimensional network of corner-sharing triangles, supporting electronic band structures with Dirac crossings and nearly flat bands with strong spin-orbit coupling. These prototype materials exhibit different magnetic ground states, such as ferromagnetic, antiferromagnetic and paramagnetic which were wildly studied these years. Defect excitations at atomic vacancies and adatoms, which are known to provide deeper understanding and reveal new physical properties of correlation topological materials, have yet to be explored in these kagome lattice materials.

As the first combination of both theoretical prediction and experimental evidence Weyl topological system with intrinsic magnetism, $Co_3Sn_2S_2$ has been discovered to exhibit novel phenomena such as surface-termination dependent topological Fermi arcs and disorder-induced elevation of intrinsic anomalous Hall conductance, making it an ideal platform to study the defect excitations and its correlation to the topological properties of the Weyl semimetal. Scanning tunneling microscopy/spectroscopy combining with spin-polarized tip is a powerful tool to characterizing the local excitations at atomic level. Prof. GAO Hongjun's research group at the Institute of Physics (IOP), Chinese Academy of Sciences (CAS) has built up solid research capacity in these two technologies and related scientific

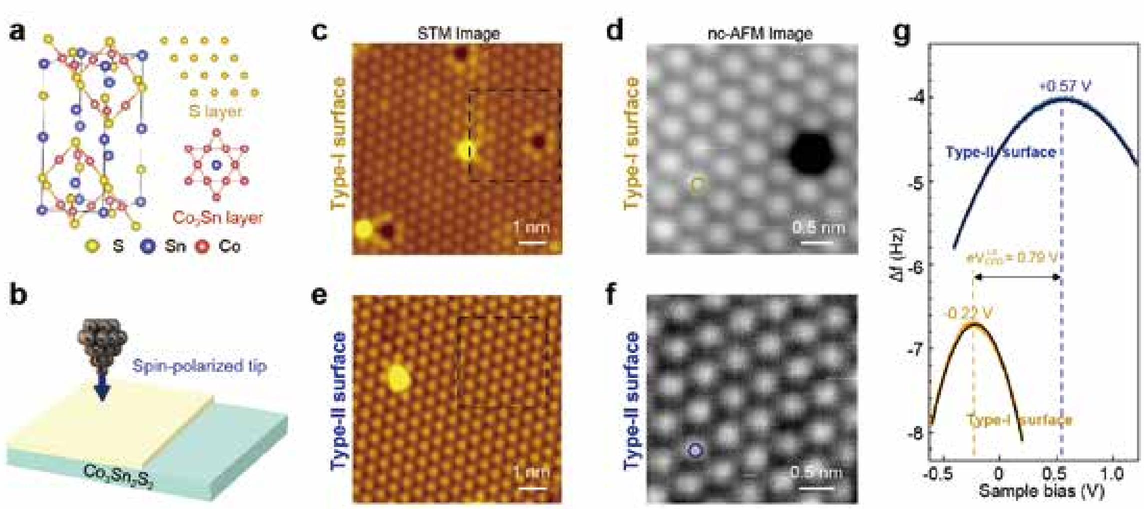

Figure 1: Identification of S-surface of Co3Sn2S2 using nc-AFM/STM

research, and has achieved a number of international top-level research results.

Recently, Prof. GAO's group, in cooperation with Prof. LIU Enke's group from IOP and Prof. WANG Ziqiang's group from Boston College, USA, first studied localized excitations from single vacancies of magnetic Weyl semimetal $Co_3Sn_2S_2$, using ultra-low temperature scanning tunneling microscopy/spectroscopy (STM/S) with spin-polarized tip and low temperature atomic force microscopy (AFM). They used non-contact AFM and local contact potential difference measurement to identify the S-terminated surface from two typical cleaved surfaces. Then they reported the discovery of bound magnetic polarons nucleated around single S-vacancies in nearly non-magnetic S surface by spin-polarized STM. The magnetic polarons emerged as bound states in the conductance map with a three-fold rotation symmetry.

Applying external magnetic fields up to ±6 T normal to the surface reveals that the binding energy of the localized magnetic polaron linearly increases as a function of the field magnitude regardless of the field direction. This anomalous response indicates dominant orbital magnetization contribution to the local magnetic moment (~ 1.35 μB). Contributed by the appreciable magneto-elastic coupling around the S-vacancy, this new excitation is termed as a localized spin-orbit polaron (SOP). The significant diamagnetic orbital magnetization has a possible topological origin associated to the diamagnetic circulating current around the S-vacancy. The SOPs observed on nearly non-magnetic atomic layer of $Co_3Sn_2S_2$ can enhance magnetism and more robust time-reversal-symmetry-breaking topological phenomena.

Given the role of magnetic dopants in dilute magnetic semiconductors, the vacancy-induced SOP

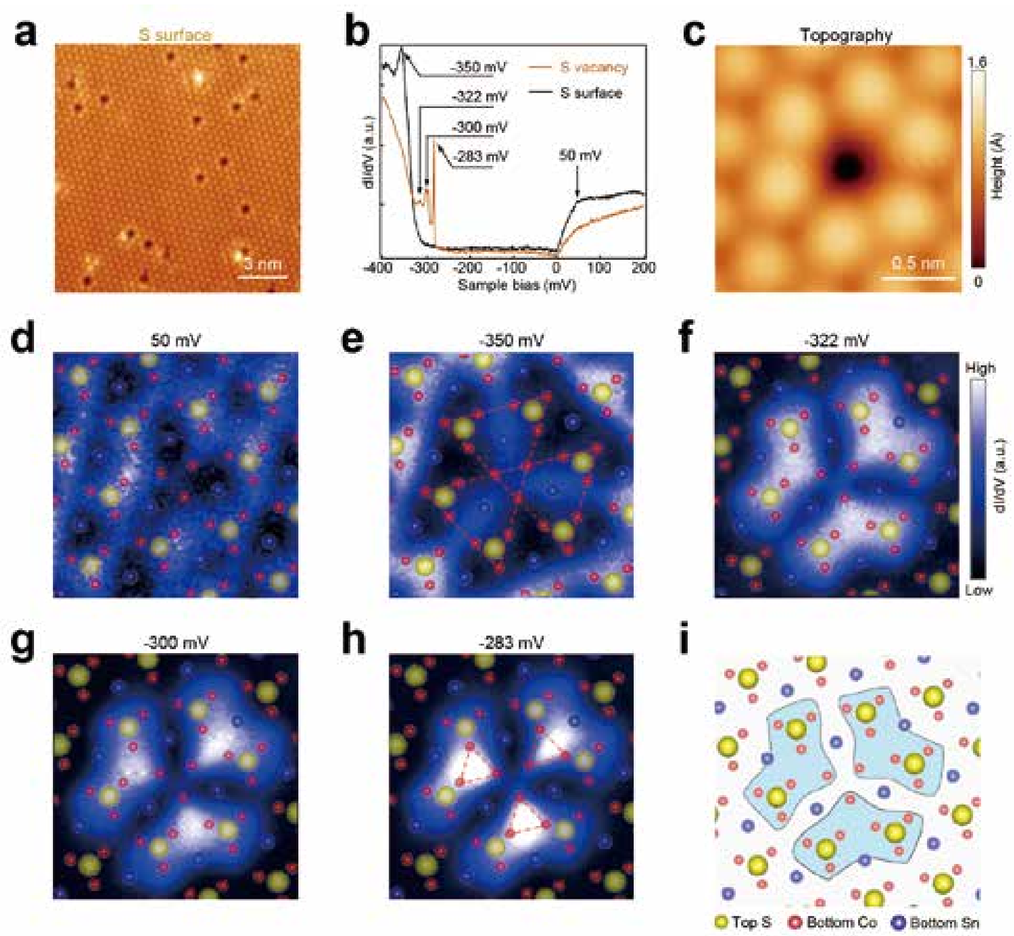

Figure 2: Localized excitations around a single S-vacancy at the S-terminated surface of $Co_3Sn_2S_2$

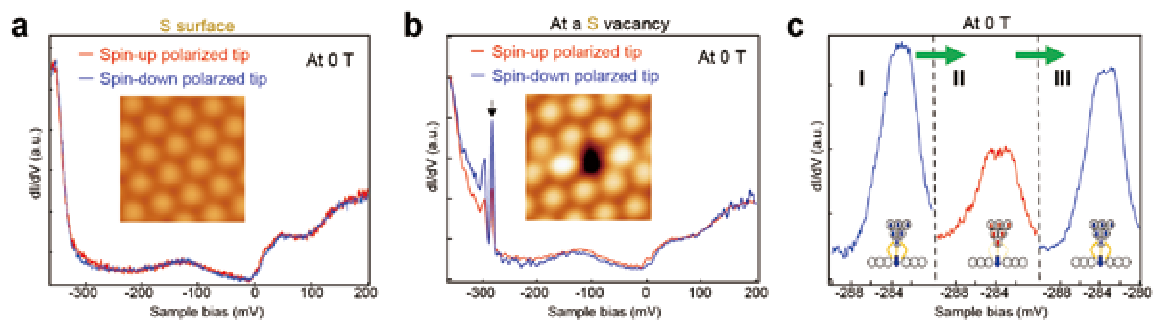

Figure 3: Spin-polarized bound states at a single S-vacancy

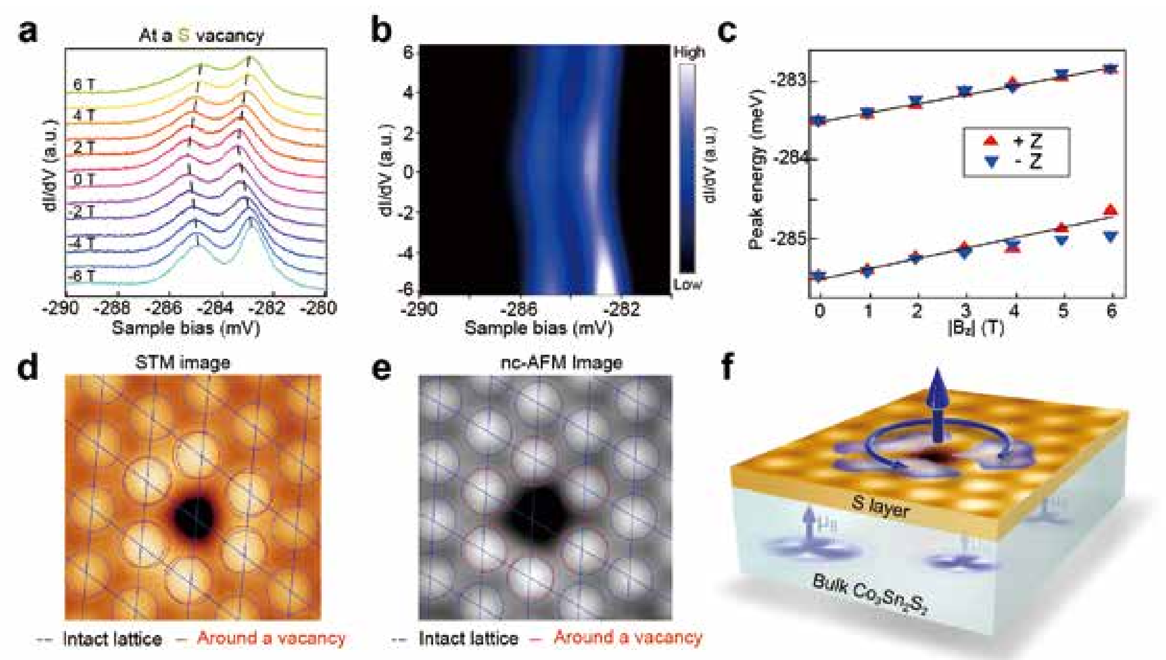

Figure 4: Anomalous Zeeman shift of the bound states and spin-orbit polaron at a single S-vacancy

may provide a new path toward generating magnetic moments in correlated nonmagnetic topological semimetals. Furthermore, the discovery of the localized SOP opens a novel route for manipulating the magnetic order and the topological phenomena in Weyl semimetal $Co_3Sn_2S_2$. Controlled engineering of the SOPs may pave the way toward practical application in functional quantum devices.

XING Yuqing, Dr. SHEN Jianlei, Dr. CHEN Hui and Dr. HUANG Li contribute equally to this work. Profs. LIU Enke, WANG Ziqiang and GAO Hong-Jun are the corresponding authors. Prof. LIU Enke and his team provided high quality crystals of $Co_3Sn_2S_2$, and Prof. WANG Ziqiang provided theoretical support.

This work was financially supported by the National Natural Science Foundation of China (61888102,11974422, 11974394), the National Key R&D Program of China (2016YFA0202300,2017YFA0206303, 2018YFA0305800, 2019YFA0308500, 2019YFA0704900), and the CAS (XDB28000000, 112111KYSB20160061). This work, entitled “Localized spin-orbit polaron in magnetic Weyl semimetal $Co_3Sn_2S_2$”, was published online in *Nature Communications* 11, 5613 (2020) on the 5th November 2020.

Link: https://www.nature.com/articles/s41467-020-19440-2

(IOP)