Research Group for Surface and Interface Science

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Surfaces and interfaces of materials including low-dimensional (D) materials such as layered materials (2D), atomic chains (1D), and clusters (0D), exhibit intriguing properties different from the bulk materials owing to the breaking of spatial inversion symmetry. The objective of our group is to explore exotic low-D materials/surfaces and hydrogen dynamics towards the development of novel functionalities at surfaces and interfaces by taking advantage of advanced quantum beams such as muons, positrons, neutrons, IR-THz photons, and ions.

In this report, we show two topics, orbital hybridization between graphene and Au surface [1] and weakly interacting quantum spin chain antiferromagnet [2], in addition to the research on hydrogen/deuterium separation with a graphene sheet [3] (Research Highlights, separate page).

Discovery of Orbital Hybridization between Graphene and Hex–Au(001) Reconstructed Surface

Graphene, a monolayer honeycomb lattice of carbon atoms, has extraordinary electronic properties such as ultrahigh carrier mobility and quantum Hall effect at room temperature. Au, a familiar noble metal, has a large spin-orbit interaction. The interface between graphene and Au is expected to have applications in spintronics devices. However, the mechanism of when and how Au modifies the electronic properties of graphene has not been clarified because the arrangement of Au atoms at the graphene-Au interfaces was often unknown. In this study, graphene was grown on the Hex–Au(001) reconstructed surface, which has quasi-one-dimensional (1D) periodicity and a well-defined atom arrangement [1]. The angle-resolved photoemission spectroscopy (ARPES) and the density functional theory (DFT) calculation revealed the band structure of graphene on the Hex–Au(001) surface, which governs the electronic properties of graphene. Previously, it was assumed that the quasi-1D periodicity of the Hex–Au(001) would affect the band structure of graphene without chemical bonding. In this study, the effect of quasi-1D periodicity was not observed to modify the band structure of graphene, as revealed by ARPES and DFT. Instead, a bandgap of 0.2 eV was observed at the crossing point of the graphene π and Au 6sp orbitals, indicating the hybridization of these orbitals. In other words, graphene and Au formed chemical bonds Through comparison with previous reports on graphene-Au interfaces, the epitaxial relation between graphene and Au and an isolated electronic structure of Au at the interface are found essential for the hybridization. The elucidation of the mechanism of hybridization between Au and graphene in this study will lead to the method to pass the spontaneous spin polarization of Au to graphene through chemical bonding. This phenomenon is expected to be utilized in spintronics devices, a research field such as next-generation energy-saving integrated circuits that utilize spin.

Magnetic gap excitations in weakly interacting quantum spin chain antiferromagnet $KCuPO_4 \cdot H_2O$

The S = 1/2 Heisenberg linear chain antiferromagnet is the simplest spin model; nevertheless it serves as a platform for various quantum many-body phenomena. In real linear chain magnets, often long-range magnetic order at finite temperatures is induced by weak interchain coupling. However, a dimensional crossover behavior can be observed by the inelastic neutron scattering (INS) measurement in a weakly interacting quantum spin chain antiferromagnet. In the INS spectrum, it is expected to observe gapped magnon excitations at lower energies and multiple magnon continuum excitations at higher energies.

We present $KCuPO_4 \cdot H_2O$ as a new weakly interacting quantum spin chain antiferromagnet [2]. The intrachain interaction J and interchain interaction $|J'|$ are estimated to be 172 K and 4.25 K, indicating that this compound has "moderately weak interchain interactions" suitable for investigation of a dimensional crossover phenomenon. A long-range antiferromagnetic order with an ordered moment 0.31 μ_B per spin occurs at T_N = 11.7 K. Both above and below T_N, at higher energies, the INS excitation is characterized by a two spinon continuum (Fig. 1(a)). At lower energies, below T_N, a spin gap is observed in the dispersive excitations (Fig. 1(b)). Our neutron scattering measurements reveal that $KCuPO_4 \cdot H_2O$ is a better candidate for a weakly interacting quantum spin chain system than previous linear chain antiferromagnets.

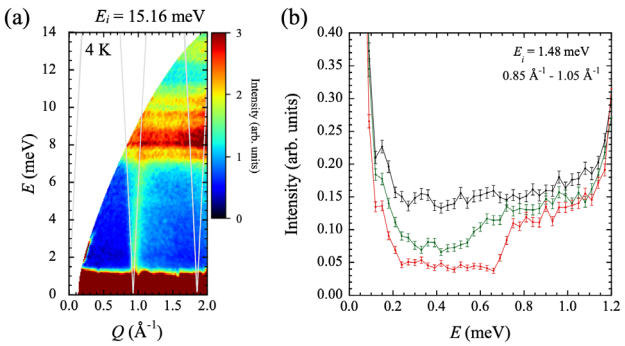

Fig. 1 (a) INS spectra at 4 K were observed with an incident neutron energy of 15.16 meV. The superimposed grey solid lines indicate the lower and upper energy boundaries of the continuum. (b) Energy dependence of the scattering integrated over Q in the range 0.85 Å^{-1} < Q < 1.05 Å^{-1}, measured at 4, 8, and 15 K.

References

[1] T. Terasawa *et al.*, Phys. Rev. Materials **7**, 014002 (2023).
[2] M. Fujihala *et al.*, Phys. Rev. B **107**, 054435 (2023).
[3] S. Yasuda *et al.*, ACS NANO **16**, 14362 (2022).