Evolution of the electronic structure of Bi_2Se_3 by hydrogen exposure

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Abstract

Bi_2Se_3 is a prototypical three-dimensional topological insulator hosting spin -momentum locked surface states. When spin current is induced on that surface, it is converted into charge current, which is known for inverse Edelstein effect [1]. This can be a promising technique for spintronics devices. Our group has developed spin-polarized hydrogen beam (SPH) [2] that is expected to inject spin current on the surface. To evaluate the mechanism of the spin-charge conversion with SPH, it is important to measure the electronic structure of topological insulators depending on the amount of hydrogen exposure, although the surface states are expected to be robust against nonmagnetic perturbations. Previous work [3] reported that atomic hydrogen exposure at 300 K selectively etches Se from Bi_2Se_3, forming Bi(111) bilayers (BLs) on the surface. However, the detailed evolution of the surface electronic structure as a function of hydrogen dose has not been systematically studied.

We performed angle resolved photoemission spectroscopy (ARPES), X-ray photoemission spectroscopy (XPS) and low-energy electron diffraction (LEED) on Bi_2Se_3 exposed to atomic hydrogen at 90 K and 300 K. Our previous study of thermal desorption spectroscopy suggested that hydrogen adsorption occurred at 300 K and that not only hydrogen adsorption but also hydrogen intercalation occurred at 90 K. ARPES results showed that the surface states were electron doped, then disappeared at high hydrogen exposure. In the case of 300 K, further hydrogen exposure resulted in the formation of Bi BL band in addition to topological surface states of Bi_2Se_3. In XPS results, doublet peaks of Bi-Bi bonding grew as hydrogen exposure increased. LEED pattern also changed from Bi_2Se_3 to Bi (111) above 600 L. In the case of 90 K, Bi BL formation did not occur indicating that the Se etching by hydrogen is an activated process.

As compared to the Se etching and the resultant formation of a Bi (111) BL surface at 300 K, the topological surface states remained up to an exposure of 60 L indicating a robust feature of the surface states.

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Atomic Structure and Dielectric Properties of a Monolayer NaBr Film on Au(001)

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Abstract

Atomic-thick dielectric films exhibit a distinct polarization mechanism. Multilayer films, including bilayers, show bulk-like characteristics because the first layer decouples the upper layer from the underlying metal substrate [1,2]. In contrast, the ions in a monolayer film are strongly influenced by the substrate, experiencing significant perturbations such as interfacial charge transfer, image-charge effects, and strain arising from lattice mismatch. This dimensional difference gives rise to the unique characteristics of the monolayer dielectric film.

In this study, we investigate the atomic structure and dielectric properties of a monolayer NaBr film grown on the reconstructed Au(001) surface using low-temperature scanning tunneling microscopy (STM), and scanning tunneling spectroscopy (STS). The NaBr islands grown on Au(001) exhibit two distinct corrugation phases: a normal phase aligned with the Au reconstruction rows along the <110> direction and a tilted phase rotated by approximately 27°. We find that the tilted phase originates from a 4.8° twist of the reconstructed Au(001) top layer. Using image potential spectroscopy and a simple parallel-plate capacitor model of the STM junction, we determine the decreased local work function (4.98 eV) and a dielectric constant (2.17) of the NaBr monolayer, which is approximately one-third of the bulk dielectric constant (6.40) [3].

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Investigation of Bonding States at the Borophane/Nickel Interface via Soft X-ray Absorption and Photoelectron Spectroscopies

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Abstract

Borophane (hydrogen boride (HB) sheets) is an atomic layered material composed of boron and hydrogen. It acts as a semimetal in its monolayer form [1], demonstrates functionality in hydrogen release [2] and as a catalyst for C-C bond formation [3], making it a promising material for diverse physical and chemical applications. Our research group has successfully produced large area borophane sheets [4], and subsequent studies have revealed significant structural changes upon heating.

In this study, we investigated borophane sheets heated at 100°C and 300°C while interfaced with nickel. The electronic states were evaluated using soft X-ray absorption spectroscopy (XAS) at the B K-edge and Ni L-edge, and soft X-ray photoelectron spectroscopy (XPS) at the B 1s, O 1s, and Ni 2p core levels. The results reveal that borophane reduces the nickel surface oxide, forming a boric oxide layer. Furthermore, we observed the formation of a nickel boride layer between the reduced nickel and the borophane.

While borophane has previously been reported to exhibit reducing properties toward transition metals [5, 6], these results suggest that borophane sheets can be used to form transition metal boride layers on various transition metal surfaces, including nickel.

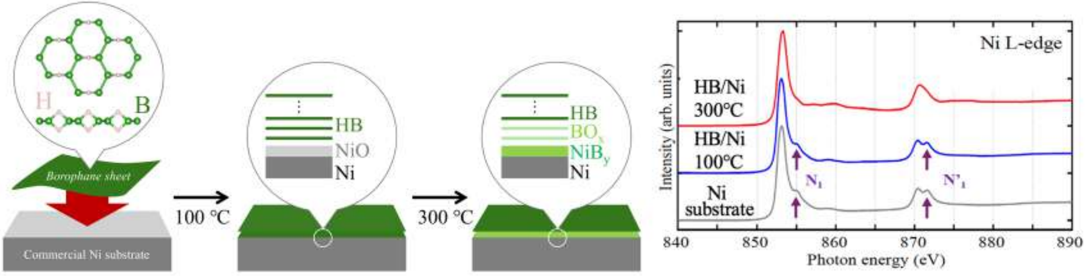

Fig. 1. Graphical abstract of this study. HB in the figure indicates borophane.

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Probing Interfacial Electronic Structure Evolution in Fe_2TiO_5/ZnO Core–Shell Nanodendrites by Soft X-ray Ptychography and X-ray Absorption Spectroscopy

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The spatially-resolved interfacial electronic/atomic structure of epitaxially grown core-shell Fe_2TiO_5/ZnO/SnO_2 [shell-Fe_2TiO_5 (FTO), core-ZnO and substrate-SnO_2 heterojunction nanodendrite (i.e FTO/ZnO/SnO_2) has been systematically investigated using synchrotron-radiation-based X-ray absorption spectroscopy (XAS), scanning transmission X-ray microscopy (STXM) combined with Ptychography, and complementary structural characterization techniques to elucidate the origin of its enhanced photoelectrochemical (PEC) performance. Detailed structural and electronic analysis reveals that lattice mismatch between FTO (020) and ZnO (002) planes primarily induces interfacial tensile strain, while the work function difference generates a built-in electric field (BIEF) via type-II band alignment. XAS analysis reveals elongation of nearest-neighbor (NN) Fe-O and Ti-O bonds, and contraction of next-nearest-neighbor (NNN) Fe-Fe, Fe-Ti and Ti-Ti bonds at the interface, indicative of interfacial tensile strain and defects in the FTO/ZnO/SnO_2. These local distortions at Fe/Ti sites along with oxygen defects, particularly at Ti sites, contribute to efficient charge separation. The Fe/Ti L_3-edge XANES STXM-Ptychography, together with O K-edge spectral modifications, disclose charge redistribution in Fe/Ti 3d (t_{2g} and e_g) states via super-exchange, which promotes spin-polarized charge transport and enhances interfacial reaction kinetics. The observed oxygen defects and orbital anisotropy in O K-edge Ptychography-XANES spectra further support efficient charge separation and facilitate directional charge transfer. This work highlights the critical roles of interfacial tensile strain, defects (oxygen vacancies/dangling bonds) and spin-charge interactions in optimizing PEC performance, offering fundamental insights into the design of advanced nanostructured heterojunctions for efficient solar water-splitting catalysts.

Keywords: Nanostructures, Heterojunction, Water Splitting, X-ray Absorption Spectroscopy (XAS), Scanning Transmission X-ray Microscopy (STXM)

STM study on tuning the Fermi level of $HfSe_2$ and V-doped $MoSe_2$

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Abstract

Controlling the Fermi level is essential for tailoring the electronic properties of semiconductors. In this work, we investigate two representative routes of chemical doping and defect control using scanning tunneling microscopy and spectroscopy (STM/STS). For V-doped $MoSe_2$, we assess the influence of substitutional V atoms on its electronic structure. Because STM primarily probes the top Se layer, the V dopants are not directly imaged. Nevertheless, STM topography exhibits dominant defect-like features whose contrast reverses with the bias polarity: they appear dark at positive sample bias and bright at negative bias. Such contrast reversal is characteristic of negatively charged acceptor states and is consistent with V atoms substituting Mo. Correspondingly, STS spectra show that the Fermi level shifts toward the valence band, indicating that V doping drives $MoSe_2$ from its intrinsic n-type nature toward p-type behavior. For $HfSe_2$, we focus on defect control via thermal annealing. STM images present the surface morphology and defect distribution, while STS measurements acquired under different annealing conditions show systematic Fermi-level shifts. The results suggest that prolonged annealing enhances the formation of selenium vacancies, which act as electron donors and move the Fermi level toward the conduction band. These results highlight the value of STM/STS in linking local defect structures with electronic properties, offering microscopic insight into how Fermi levels can be tuned through doping and defect engineering.

Step conductivity of Pb monolayers formed on Si(111) studied by low temperature scanning tunneling potentiometry

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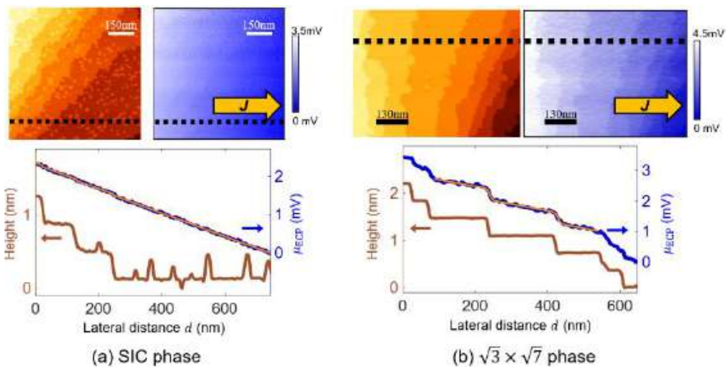
Abstract

Surface steps of a substrate play an important role on electronic and electrical properties of monolayer (ML) two-dimensional (2D) metals formed on it. Their influence has been evaluated in several ways. Through the observation of vortices on ML 2D superconductors, it is known that atomic steps work as a Josephson junction, and the degree of disruption depends significantly on metallic layers [1, 2]. In addition, surface transport measurements have revealed electrical resistance at atomic steps.

In order to quantitatively evaluate the resistance of surface steps, we utilized low-temperature scanning tunneling microscopy/potentiometry (LT-STM/P). STP allows us to obtain topographic images with nanometer-scale spatial resolution and electrochemical potential images with microvolt resolution, enabling us to correlate local transport properties with surface atomic structure [3].

We performed LT-STM/P on Pb ML reconstructed structures formed on Si(111), which are well-known two-dimensional superconductors, and revealed that in the striped incommensurate (SIC) phase (Pb coverage: 1.3 ML), the potential drop at the atomic step was sufficiently small compared to that on the terrace (Fig. (a)), suggesting weak resistance at the steps. In contrast, in the $\sqrt{3}\times\sqrt{7}$ phase (1.2 ML), a significant potential drop was observed at the steps (Fig. (b)), indicating that the steps act as stronger disorder. The distinct difference in the observed step resistance is consistent with the vortex behavior.

We quantitatively evaluated the role of surface steps through both vortex behavior and local transport measurements, demonstrating a clear correlation between the two different methods.



(a) SIC phase

(b) $\sqrt{3}\times\sqrt{7}$ phase

Figure: STP results on (a) SIC phase and (b) $\sqrt{3}\times\sqrt{7}$ phase. (upper left) topographic image. (upper right) electrochemical potential image. (bottom) cross-sectional profiles taken along the dashed lines in the upper images. The orange line is a fitted curve with a sigmoid function.

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Thermal Annealing Process, Water Storage, and Water Permeation Application of Graphene Oxide Membranes

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The in-situ environmental experiment is important to monitor the chemical de-oxidation and re-modification of reduced graphene oxide (rGO) due to the controllable adjustment of the surface functional groups of graphene oxide (GO). For scientific purposes, a perfect hexagonal ring of gra-phene (G) that exhibits various oxidation sites is crucial for inducing different chemical bonding responses and is effective for external gas molecules. A membrane composed of G/GO/rGO mate-rials has been fabricated for potential energy and electrical applications, as described in the report. Using ambient pressure X-ray photoelectron spectroscopy (AP-XPS), we observe the thermal evolu-tion and re-oxidation behavior of thermally reduced graphene oxide (Th-rGO) under various at-mospheric and humidity conditions. The thermal process was heated from room temperature to 300 °C in increments of 50 °C under ultra-high vacuum (5×10^{-6} mbar) and in simulated air (0.6 mbar, 80% N_2 / 20% O_2), in order to introduce the thermal energy and gas interaction into the GO mem-brane. In a vacuum environment (Th-rGO-Vac), the C–O–C and C=O groups decompose primarily as the temperature increases. Meanwhile, the C-OH and O=C–OH groups have higher ratios at low-er temperatures, but these ratios decrease after reaching 150°C. In a simulated air environment (Th-rGO-Air), C–O–C, C=O, and C-OH also decompose directly, but only the O=C–OH group has a crossover behavior during the thermal annealing process. In the water storage application, following thermal annealing in ultra-high vacuum and simulated air, an increase in water gas pressure (0.1–0.6 mbar) was applied to the same Thr-GO membranes during the AP-XPS experiment. The pro-nounced chemical bonding and bonding transfer have been observed in both the Th-rGO mem-brane with rising vapor pressure, primarily through the formation of C-O-C and C–OH groups. Even at pressures as low as 0.1 mbar, the surface of Th-rGO-Air is already saturated with adsorbed water molecules, highlighting strong water–surface interactions. In contrast, the Th-rGO-Vac mem-brane offers higher water gas storage and better chemical bonding states than the Th-rGO-Air, mak-ing it suitable for recyclable energy applications. AP-XPS experiments were conducted using the liquid cell membrane, with the main chamber maintained under ultra-high vacuum and at three dif-ferent nitrogen pressures (0.1, 0.3, and 0.6 mbar). The key aspect is to determine the rate of water molecule permeation through the GO membrane based on the pressure gradients between the main chamber and the liquid chamber. These findings reveal the crucial role of atmospheric gases and water vapor in modulating the surface chemistry and electronic properties of rGO, offering insights for sensing and electronic tuning applications.

Keywords: Graphene Oxide, Thermal reduction, Ambient Pressure - XPS, Re-oxidation, Humidity response

Tunable plasmonic and intraband transitions of single Ag_2Se quantum dots via photo-induced force microscopy

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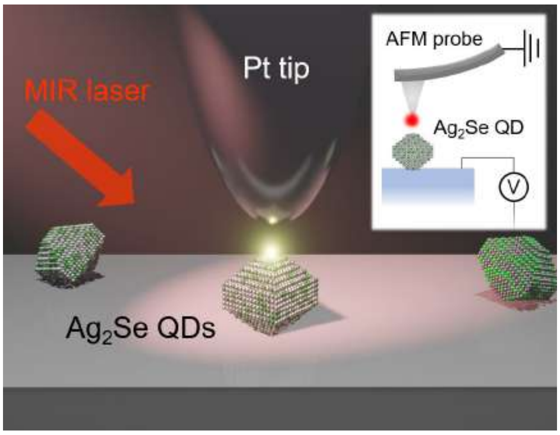
Abstract

Quantum dots (QDs) occupy an intermediate regime between bulk solids and individual atoms or molecules, exhibiting size-dependent and discrete energy levels. While most studies have focused on interband transitions across the bandgap, intraband transitions within the conduction or valence bands remain less explored. Here, we use photo-induced force microscopy (PiFM)[1] to directly probe individual self-doped Ag_2Se QDs[2] at the single-dot level. PiFM spectra reveal a clear size-dependent evolution at the single-dot level: smaller QDs (AFM height $h \leq 9$ nm) display coexisting intraband ($1S_e$ to $1P_e$) and quantum plasmon resonance (QPR) features, whereas larger QDs ($h \geq 10$ nm) predominantly show QPR signatures with stronger photo-induced dipole force (PiDF) and size-dependent resonance shifts. In addition, we applied an external bias to the QDs to manipulate these responses. Under a small bias potential, we observe reversible variation of the intraband and QPR responses. Beyond a threshold voltage, on the other hand, the spectra abruptly changed, which can be attributed as field- and thermal-driven phase transitions. Together, these results provide insight into the size-dependent mid-IR responses in self-doped Ag_2Se QDs and establish PiFM as a versatile platform to investigate nanomaterials.



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Spin-polarized Fermi surface of Tl bilayer crystal formed on Ag(111)

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Abstract

Atomic layer crystals formed on solid surfaces show spin-polarized electronic bands originating from the combination of spin-orbit coupling and spatial inversion asymmetry. In case of atomic layer superconductor, novel physical properties emerging from the concert of electron spin and superconductivity are expected. In contrast to thallium (Tl) atomic layers formed on Si(111), which show spin-polarized bands but no superconductivity in case of single Tl layer [1,2] and show superconductivity but no spin-polarized band in case of Tl bilayer [3,4], Tl bilayer formed on Ag(111) (BL-Tl/Ag) is reported to show spin splitting at the $\overline{\mathrm{K}}$ point of the Brillouin zone and to become superconducting at below 0.92 K [5]. In this presentation, we report the spin polarization in the Fermi surface of BL-Tl/Ag obtained by spin- and angle-resolved photoelectron spectroscopy (SARPES). Based on the SARPES and theoretical calculation results, we will discuss the origin of the novel spin-polarized Fermi surface of BL-Tl/Ag in more details.

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Characterization of interfaces between contact metals and monolayer 2D semiconductor

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Abstract

Transition-metal dichalcogenides (TMDs), as members of the two-dimensional (2D) material family, exhibit strong potential for next-generation semiconductor applications. However, the complex interfacial mechanisms between TMDs and metals, including orbital hybridization and interface dipole redistribution often lead to unfavorable contact resistance, which in turn increase energy consumption and degrades overall device performance. This highlights the need for a comprehensive and systematic investigation of ML-TMD to metal interfaces.

In this work, we have studied the interfacial properties of both metal-TMD and semimetal-TMD systems using scanning tunneling microscopy/spectroscopy (STM/s), X-ray photoelectron spectroscopy (XPS) and density functional theory (DFT) calculations. By studying monolayer MoS_2 and WS_2 on a variety of metals, we uncover a consistent band-gap-reduction behavior across different contact configurations, arising from orbital hybridization at the interface. In addition, Fermi-level shifts observed in our measurements indicate doping effects induced by interlayer charge transfer. Overall, our work provides complementary guidelines for selecting optimal contact materials for future semiconductor technologies.

Overview of Capabilities, Experiments and Recent Advances at the SPring-8 Angstrom Compact Free Electron Laser (SACLA)

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Abstract

X-ray free-electron lasers, like Japan’s SPring-8 Angstrom Compact Free Electron Laser (SACLA), with their ultrashort X-ray flashes, extremely high brilliance nanometer focus, have by now been known to reveal new avenues and novel techniques for exploring different material properties as well as various phenomena. Their ability to generate extremely short but highly intense X-ray flashes sets X-ray free-electron lasers (XFEL) apart from their more established synchrotron counterparts. Owing to the ultrashort X-ray pulse and exceptionally stable synchronization with the optical laser system, SACLA provides an exceedingly high time resolution of 50 fs. In addition, due to the extremely high X-ray intensity, nonlinear X-ray absorption effects, such as soft X-ray second-harmonic generation (SXSHG), can be achieved. SXSHG is a highly versatile technique as it combines sensitivity to regions of inversion symmetry breaking, such as at surfaces and interfaces, with element specificity of core resonance X-ray absorption [1]. Furthermore, it is possible to separate the crystalline and magnetic contributions to inversion symmetry breaking by applying a reversible magnetic field and disentangling the even and odd signal components under field direction reversal [2]. The penetration depth of the XUV range enables the overlying layer to be penetrated, allowing selective investigation of both sides of buried interfaces in various functional heterostructure samples.

In this talk, I will present our group's recent advances in the development of novel measurement techniques at the soft X-ray beamline BL1 of SACLA, specifically with the focus on SXSHG. We have recently focused on developing tools to establish ultrafast time-resolved SXSHG experiments. By synchronizing SACLA’s ultrashort X-ray flashes with femtosecond laser pulses, we exploit the femtosecond time resolution to resolve ultrafast demagnetization processes, spin and charge transfer, as well as additional forms of energy transfer across interfaces. Utilizing the element specificity, we aim to selectively probe and separate the dynamics on either side of the buried interfaces with femtosecond resolution. The capabilities of SACLA to generate extremely high intensity femtosecond X-ray flashes uniquely position us to utilize time-resolved SXSHG to investigate the ultrafast dynamics at buried interfaces in complex heterostructures.

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Angle-Dependent Carrier Transport at the Bi/MoS_2 Interface: Correlation Between Experimental Observations and Theoretical Analysis

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The electrical transport properties of two-dimensional (2D) material-based heterostructures are highly sensitive to lattice alignment and interfacial coupling. In this work, we systematically investigate the angle-dependent conductivity and carrier mobility at the bismuth (Bi)–molybdenum disulfide (MoS_2) interface. By controlling the rotational alignment between the Bi contact and MoS_2 channel, both experimental measurements and theoretical simulations reveal significant modulation in transport characteristics. The conductivity exhibits a remarkable ~5.8× enhancement when the rotation angle decreases from 30° to 0°. These results indicate that precise control of interlayer twist angle can effectively tailor interfacial coupling strength and electron injection efficiency. Simulation results further demonstrate that the twist angle significantly influences carrier injection and the corresponding transmission distribution, with the 0° configuration yielding the highest transmission and the 30° configuration the lowest. These findings confirm that lattice-matching engineering provides an effective strategy for tuning interfacial coupling strength and electron injection efficiency, offering a promising route toward optimizing device performance in future heterogeneous integrated circuits to enhance both power efficiency and computational speed.

Keywords: Two-dimensional material, Contact engineering, Twist angle-dependent, Transition-metal dichalcogenides

Magnetic Coupling in Metal–Organic Structures on a 2D Superconductor: A Comparison of $FeDCA_3$ and $NiDCA_3$ on $NbSe_2$

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Abstract

Two-dimensional metal–organic structures that form ordered magnetic lattices on a superconducting substrate provide a unique platform to study the interplay between magnetic ordering and superconductivity. In this work, we investigate Fe- and Ni-based dicyanoanthracene ($FeDCA_3$, $NiDCA_3$) structures on $NbSe_2$ to explore the magnetic coupling in this system and to understand how it is influenced by both the molecular linkers and the superconducting substrate.

Using scanning tunneling microscopy (STM), X-ray absorption spectroscopy (XAS), and X-ray magnetic circular dichroism (XMCD), we observed weak magnetic anisotropy of ~ 0.1 meV and Heisenberg-type antiferromagnetic interactions between Ni centers in $NiDCA_3$ with a Curie-Weiss temperature of -2.5 K, which result from competing contributions: super-exchange via the molecular linkers and Ruderman–Kittel–Kasuya–Yosida (RKKY) interactions mediated by the conduction electrons of the substrate [V. Vaňo et al., Phys. Rev. Lett. **133**, 236203 (**2024**)]. Conversely, in the isostructural $FeDCA_3$ we find a strong out-of-plane anisotropy of the order of ~ 10 meV but with a three-times smaller antiferromagnetic coupling of Ising-type, indicating that the effect of the interaction between the Fe 3d orbitals and the molecular ligand is mainly to lift the degeneracy of the spin multiplet. Our work reveals the dual role of organic coordination and substrate coupling in determining the overall magnetic behavior of metal-organic structures on superconductors.