Role of the surface state in the Kondo resonance width of a Co single adatom on Ag(111)

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We address the long-term controversy on the fundamental question of the role of the surface state on the Kondo effect with Co adatoms on a Ag(111) surface. The width of the Kondo resonance oscillates with the same period of half Fermi wavelength of the surface state. But the amplitude increases for a Co adatom placed next to another Co adatom, at the vicinity of a step edge, and quantum confined within nanocorrals. A greater than three times enhancement of the resonance width can be achieved when quantum confinement is introduced. The experimental results are described quantitatively utilizing an analytical model where the contributions of the bulk and surface states are weighted by their exchange values with the magnetic impurity. These findings clarify the role of the surface state on the Kondo effect and pave a pathway to tailor the Kondo effect via quantum confinement of the surface state.

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I. INTRODUCTION

The Kondo effect was discovered as a temperature-dependent resistivity minimum in gold in the 1930s [1]. Its origin, however, remained a puzzle for ∼30 years until Kondo calculated that the scattering rate of conduction electrons by a magnetic impurity should increase with decreasing temperature [2]. Besides the resistance minimum, other effects such as heat capacity and susceptibility anomalies were also found [3,4]. With advances of nanotechnology, it becomes possible to investigate the Kondo effect down to a single atomic or molecular level [5–10]. Low-temperature scanning tunneling microscopy (LT-STM) is a powerful tool to study the effect due to its high spatial resolution, spectroscopy capability, and low-temperature environment. At low temperature, the local spin of the magnetic impurity is screened due to the formation of a spin-compensated cloud of conduction electrons, resulting in a spectroscopic signature near the Fermi level. This is the Kondo [2] or Abrikosov-Suhl resonance [11,12], where the Kondo temperature T_K, is proportional to the resonance width $w = k_B T_K$, and k_B is the Boltzmann constant.

As the Kondo effect is related to the exchange of a local spin and the electrons at the Fermi level, E_F, it correlates with the local density of state (LDOS) at E_F, $\rho(E_F)$, namely, $k_B T_K = D \exp[-1/J\rho(E_F)]$ [11–16], where D is the band cutoff and J is the exchange constant. When a surface state crosses the Fermi level, it also contributes to $\rho(E_F)$. It is thus anticipated to influence T_K. The fundamental questions on whether and how the surface state influences the Kondo temperature, however, still remain as an ongoing debate [9,17–29]. For example, Knorr *et al.* compared the spatial attenuation of the amplitude of the Co Kondo resonance on Cu(111) and Cu(100) and found almost the same decay length [18], and thus concluded that the surface state plays only a minor role. However, Merino and Gunnarsson compared the same experimental data with theoretical calculations and reported that the attenuation became surfacelike when the horizontal distance is >0.3–0.5 nm [19]. Lin *et al.* investigated this problem twice reaching different conclusions [20,21]. Limot and Berndt compared the measured value of w for a Co adatom placed at different locations near a step edge on Ag(111) and found no apparent change, suggesting a minor role for the surface state [26]. By investigating the Kondo effect of the Co adatom on Ag(111) terraces with different widths, Henzl and Morgenstern reported that the surface state does influence the decay behavior of the Kondo resonance but not T_K [27].

To address this controversy, we performed systematic studies of the Kondo resonance for Co monomers on Ag(111) and found compelling evidence that the surface state does influence the Kondo temperature. Kondo temperature oscillations with increasing amplitude are found for the three cases studied of a Co adatom (i) placed next to another Co adatom, (ii) at the vicinity of a step edge, and (iii) quantum confined within nanocorrals. Our findings can be understood by an analytical model where the contributions of surface and bulk states are weighted by their exchange values with the Co adatom, J_b and J_s. Within the model, J_b and J_s are derived consistently for all three cases. Our findings also demonstrate an approach to control the Kondo effect via the local modification of the LDOS of the surface state. In comparing with previous methods [7,8,15,30–35], our approach has the advantage that the Kondo effect can be continuously tuned with large magnitude, thus providing new opportunities in spintronics and spin-based quantum information processing.

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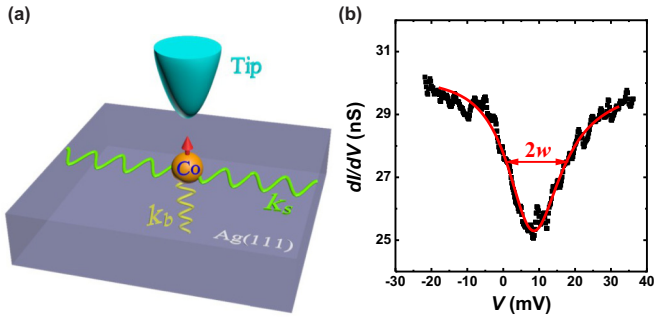

FIG. 1. (a) Sketch of the Kondo resonance measurement with a STM in the presence of both bulk and surface states. (b) Typical Kondo resonance curve measured for a single Co adatom on a wide Ag(111) terrace at 4.7 K ($V_b = 50$ mV and $I = 1$ nA). Red curve is the fitting that utilizes Eq. (1).

II. EXPERIMENTAL DETAILS

The experiments were performed in an ultrahigh vacuum chamber (2×10^{-11} mbar) equipped with a LT-STM and a sputter gun. The Ag(111) crystal was cleaned by cycles of argon ion sputtering (at 1.5 keV) and annealing (at 870 K). High-purity Co were deposited at the STM stage with a typical rate of 0.002 monolayer/min by means of electron beam evaporation at ~6 K. Tungsten tips, formed by electrochemical etching and *in situ* electron beam heating, were used [36]. The bias voltage V_b refers to the sample voltage with respect to the tip. The typical scanning conditions are tunneling current $I =$ 1 nA and $V_b = 50$ mV at 4.7 K. Spectroscopy measurements were performed via the modulation technique utilizing an amplitude (V_{mod}) of 2 mV and a frequency of 6.3 kHz after stabilizing the tip at 50 mV and 1 nA unless specified. We used atomic manipulation [37] to move the Co adatom with the condition of positioning the tip ~0.3 nm closer to the sample after stabilizing at −0.5 V and 1 nA. As the tip might change during the atomic manipulation process, we formed our tip until a steplike surface state spectrum (see Fig. S1 in Supplemental Material [38]) was obtained on top of a wide terrace before measuring the Kondo resonance each time.

III. RESULTS AND DISCUSSIONS

Figure 1(a) shows a sketch of the experiments. Typically, STM measurements are sensitive to the bulk state with the wave vector of $\vec{k}_b$. On a noble metal (111) surface, such as Ag(111), there is a surface state crossing the Fermi level and can contribute to the tunneling current [46]. When a Co monomer is placed on a Ag(111) surface, a Kondo effect appears as a resonance. A typical resonance curve is presented in Fig. 1(b). It shows an inverse peak centered at ~8 meV above E_F. Following Refs. [10,35,47], we fitted our dI/dV spectra with Fano formula to obtain w:

$$\frac{dI}{dV} = a\frac{[q+\varepsilon(V)]^2}{1+\varepsilon(V)^2} + bV + c \quad \text{with} \quad \varepsilon(V) = \frac{eV-\varepsilon_0}{w}. \tag{1}$$

In it, a represents the resonance amplitude, and b and c are the linear and constant background. Meanwhile, q represents the line shape of the resonance, and ε_0 is the shift of the resonance from E_F. We chose the fitting range of $\sim 4w$ for here and the rest of Kondo resonance width fitting. The fitting yields 8.3 ± 0.2 meV, $q = -0.09 \pm 0.01$, and $\varepsilon_0 = 7.8 \pm 0.2$ meV for a Co monomer on a wide Ag(111) terrace, consistent with previous investigations [25–27,48]. We also measured the resonance amplitude as the function of lateral tip-adatom separation and found similar decay behavior as reported in Ref. [19].

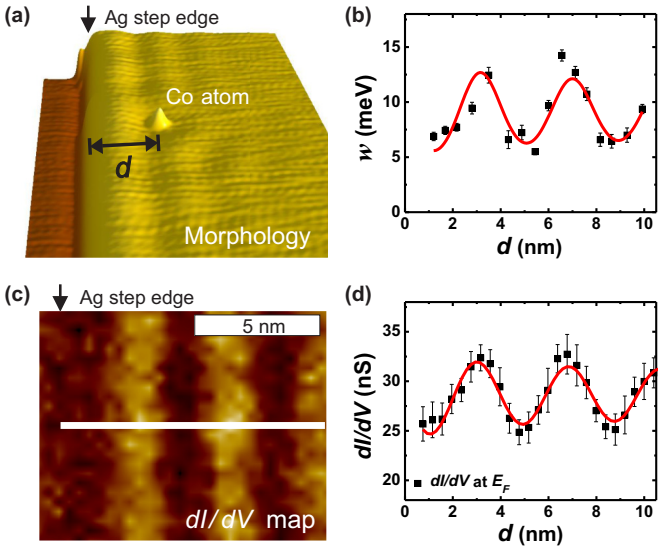

FIG. 2. (a) Topographic view of a single Co adatom with a separation d from the step edge. (b) d-dependent Kondo resonance width. The estimated statistical error margin for three times repeating measurements is approximately two to three times the error margin obtained from the fitting. (c) Experimentally obtained dI/dV mapping at the Fermi level (at −0.1 meV) near the same step edge after removing the Co adatom. (d) The line profile across the step edge as marked in (c). Red curves are fittings (see text). In all measurements, $V_b = 50$ mV and $I = 1$ nA.

We investigated the Kondo effect of a single Co adatom near a step edge, where the modulation of LDOS caused by the scattering of the surface state has been studied previously [46,49]. Figure 2(a) shows a typical morphology of a Co adatom placed on the upper terrace with a separation d from the step edge. We performed spectroscopy measurements on top of the Co adatom as a function of d (see Fig. S2 in the Supplemental Material for representative spectra [38]). The experiment is similar to the one reported by Limot and Berndt [26] but our investigation was performed with a much wider d range. We fitted the Kondo resonance curves with Eq. (1), and plot w vs d in Fig. 2(b). We note that the step edge may cause a nonlinear dI/dV background. To minimize this influence on the Kondo resonance width fitting, we fitted our data with different fitting ranges and only used the data which shows little variations (see Part 3 of Supplemental Material [38]). The d-dependent w exhibits a strong oscillation with an amplitude of ~7 meV. The oscillation period, ~3.8 nm, is identical to the half Fermi wavelength of the Ag(111) surface state, $\lambda_{E_F}/2$. To identify the correlation of the variation of w with the LDOS, we moved the Co adatom away and performed the dI/dV mapping at E_F with the result shown in Fig. 2(c).

The line profile across the step edge, Fig. 2(d), shows a strong oscillation also with a period of 3.8 nm and an amplitude of ~6 nS. Since the bulk state is position independent, a constant value of w would be expected if the Kondo resonance were formed by the bulk state only. Our finding of strong Kondo temperature oscillation with a period of $\lambda_{E_F}/2$, therefore, demonstrates that the surface state does contribute to the Kondo resonance. We note that our result is not in contradiction to the experiment of Limot and Berndt [26]. In the d range they investigated, 0.8–2.4 nm, our measured w values also show little variation [Fig. 2(b)]. We note that the oscillations of w are well reproduced [see Fig. S5(a) in the Supplemental Material [38]].

To understand our findings, we followed the Anderson impurity model [50] and took into account contributions of both the bulk and surface states. Given the orthogonality of these two states, the total hybridization energy Δ is the sum of the bulk-adatom and surface-adatom hybridization energies, namely, $\Delta = \Delta_b + \Delta_s$, with $\Delta_b = \pi \sum_{\vec{k}_b} |V_{\vec{k}_b d}|^2 \delta(E_F - E_{\vec{k}_b})$ and $\Delta_s = \pi \sum_{\vec{k}_s} |V_{\vec{k}_s d}|^2 \delta(E_F - E_{\vec{k}_s})$. $E_{\vec{k}_b}$ and $E_{\vec{k}_s}$ are the energies of the bulk and surface state electrons, respectively. $V_{\vec{k}_b d}$ and $V_{\vec{k}_s d}$ are the hybridization matrix elements. When the band cutoff of both surface and bulk states are close, the Kondo temperature in the hybridization energy form can be written as $k_B T_K = \tilde{D} \exp(-\pi |\varepsilon_d||\varepsilon_d + U|/U\Delta)$ [14]. $\tilde{D}$ is the effective band cutoff, ε_d is the d level with respect to E_F, and U is the Coulomb energy for the double occupancy of the impurity state. We note that the using of a single effective band cutoff is an approximation, and more rigorous theory such as first-principles or Green's function based calculations may be needed for systems possessing both bulk and surface bands. If we treat both $V_{\vec{k}_b d}$ and $V_{\vec{k}_s d}$ as constants, the hybridization energy is $\Delta_b = \pi |V_b|^2 \rho_b(E_F)$ and $\Delta_s = \pi |V_s|^2 \rho_s(E_F)$. $\rho_b(E_F)$ and $\rho_s(E_F)$ are the bulk and surface LDOS at E_F, respectively (shortened to ρ_b and ρ_s hereafter). With the Schrieffer-Wolff transformation [51], we can further obtain the Kondo resonance width as

$$w = k_B T_K = \tilde{D} \exp\left(-\frac{1}{J_b \rho_b + J_s \rho_s}\right). \tag{2}$$

Since the variation of the LDOS is caused by lateral scattering of the electrons, the LDOS near a step edge can be generalized into the following form [29,52]:

$$\begin{aligned} dI/dV &= B\rho_b + S\rho_s(x) \quad \text{with} \\ \rho_s(x) &= \rho_{s0}[1 + A\cos(2kx + \delta_1)/(kx)^\alpha], \end{aligned} \tag{3}$$

where B and S are tunneling factors for bulk and surface electrons, respectively. ρ_{s0} is the surface LDOS on a clean and wide terrace ($x \to \infty$). (The variable x refers to d in this configuration.) The remaining parameters are the wave number k, the oscillatory amplitude A, the phase shift δ_1, and the decay constant α. Utilizing Eqs. (2) and (3), we can further derive that

$$w = \tilde{D} \exp\left\{-\frac{1}{J_b \rho_b + J_s \rho_{s0}[1 + A\cos(2kx + \delta_1 + \delta_2)/(kx)^\alpha]}\right\}. \tag{4}$$

To accommodate the additional perturbation caused by the Co adatom used for probing the Kondo effect, an additional phase shift δ_2 is introduced.

We used Eq. (3) and the experimentally obtained dI/dV shown in Fig. 2(d) to fit the LDOS. The fitting (red curve) reproduces the experimental result. In it, the LDOS of both the bulk and surface states of Ag(111) are incorporated as follows. Using the measured effective mass $m^* = 0.42 m_e$ [46] and the lattice constant of 0.408 nm, we obtain $\rho_{s0} = 0.125$ (1/eV). We further take $\rho_b = 0.27$ (1/eV) [53] and perform the fitting. The results are listed in the central column of Table SI in the Supplemental Material [38]. The k value agrees with the Fermi wave vector of the surface state, 0.83 (1/nm) [54]. B and S are STM tip dependent but consistent values are obtained when the same tip is used. A, α, and δ_1 are terrace width dependent but show weak variation for terrace widths >50 nm. To extract J_b, J_s, δ_2, and $\tilde{D}$, we used the above values and Eq. (4) to fit the measured w in Fig. 2(b). The fitted result (red curve) reproduces the experimental data. The fitting yields $J_b = 0.46 \pm 0.05$ eV, $J_s = 0.33 \pm 0.10$ eV, $\delta_2 = -0.25 \pm 0.19$ rad, and $\tilde{D} = 5.36 \pm 1.42$ eV. The obtained $\tilde{D}$ is close to the reported bulk band cutoff of 5 eV [55], suggesting the band cutoff of the surface and bulk states are similar and validating the approximation of the model that we have taken. We note that Ref. [46] pointed out that there could be a phase shift existing in between the LDOS and the experimentally obtained dI/dV when a small bias voltage is used. Following the same method, we analyzed this phase shift and found it may induce an enhanced δ_1 and reduced δ_2 by ~0.4 rad. But the other parameters remain almost the same within the error margin.

To further confirm our experimental findings and the validity of the above analysis, we also performed studies for a Co adatom placed at the vicinity of another Co adatom (twin-atom case) and quantum confined within nanocorrals. As the LDOS modification caused by a single adatom is generally smaller than that induced by a step edge, a weaker oscillation of w is expected. On the contrary, a stronger oscillating behavior should be found when a Co adatom is quantum confined within nanocorrals due to the stronger variation of the LDOS [17,56–59]. Meanwhile, the oscillations should have the same period of $\lambda_{E_F}/2$ of the surface state, and the fitted values for J_b and J_s should be the same.

Figure 3(a) shows the typical topographic image of the twin-atom case. We performed the Kondo resonance study on top of both Co adatoms as a function of their separation l. The spectra are similar to the one shown in Fig. 1(b). The result, w vs l, is plotted in Fig. 3(b). Almost the same resonance widths are obtained on top of both atoms, suggesting the high accuracy of the measurements. Indeed, a much weaker l-dependent w oscillation is found [see Fig. S5(b) in the Supplemental

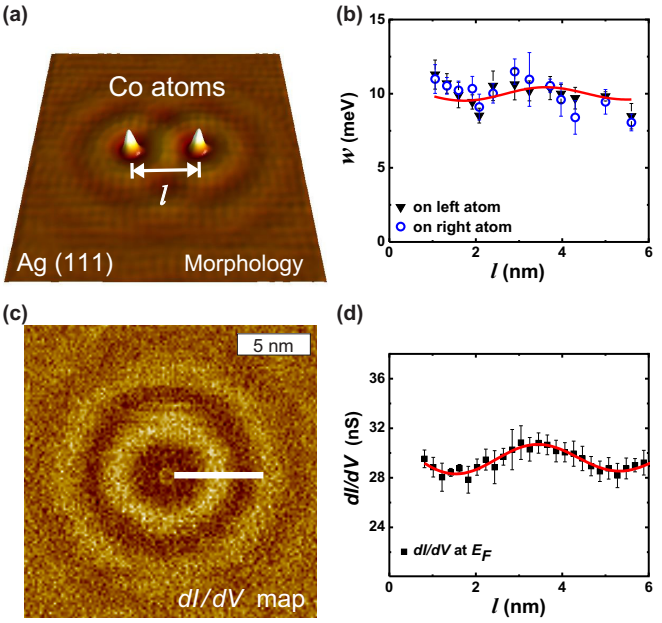

FIG. 3. (a) Topographic view of two Co adatoms separated with distance l and on a wide Ag(111) terrace. (b) l-dependent Kondo resonance width obtained on top of both adatoms. (c) The experimentally obtained dI/dV mapping at E_F (-0.1 meV) within the vicinity of a single Co adatom. (d) Line profile of dI/dV as marked in (c). Red curves are fittings (see text). In all measurements, $V_b = 50$ mV and $I = 1$ nA.

Material [38] for the data reproducibility]. Accordingly, we removed one of the Co adatoms and performed the dI/dV mapping near E_F, shown in Fig. 3(c). A line profile, as marked in Fig. 3(c), also shows an oscillation [Fig. 3(d)]. The amplitude of $\sim$2 nS is smaller than the one caused by the step edge. Importantly, we also found both l-dependent w and dI/dV at E_F share the same oscillating period of $\lambda_{E_F}/2$, consistent with the results near the step edge.

Figure 4(a) shows a typical circular corral formed by Co atoms with a Co adatom placed at the center, noted as the Co-centered corral. We measured the dI/dV spectra on top of the Co adatom located at the center. After that, we removed the center Co atom and performed the dI/dV measurements at the center of the empty corral [Fig. 4(b)]. By repeating the same strategy, we obtained the dI/dV spectra at the centers of both Co-centered and empty corrals with radius r varied from $\sim$2.9 to $\sim$10.2 nm. The representative curves are shown in Figs. 4(c) and 4(d). Figure 4(e) summarizes the r-dependent w extracted from Fig. 4(c). A much stronger oscillation of w is found in comparison with the case near the step edge. The maximum value reaches 25.1 meV (corresponding to a Kondo temperature of $\sim$291 K), which is about three times the value obtained for a single Co monomer on a wide terrace. The oscillation period is again $\sim$3.8 nm. The finding of Kondo resonance width oscillations with the same period but increasing amplitude for a Co adatom placed within the vicinity of another adatom, near a step edge and within nanocorrals demonstrates the surface state does influence the Kondo effect. The value of the dI/dV spectrum at E_F measured in the center of the empty corrals [see vertical dashed line in Fig. 4(d)] as a function of r is plotted in Fig. 4(f).

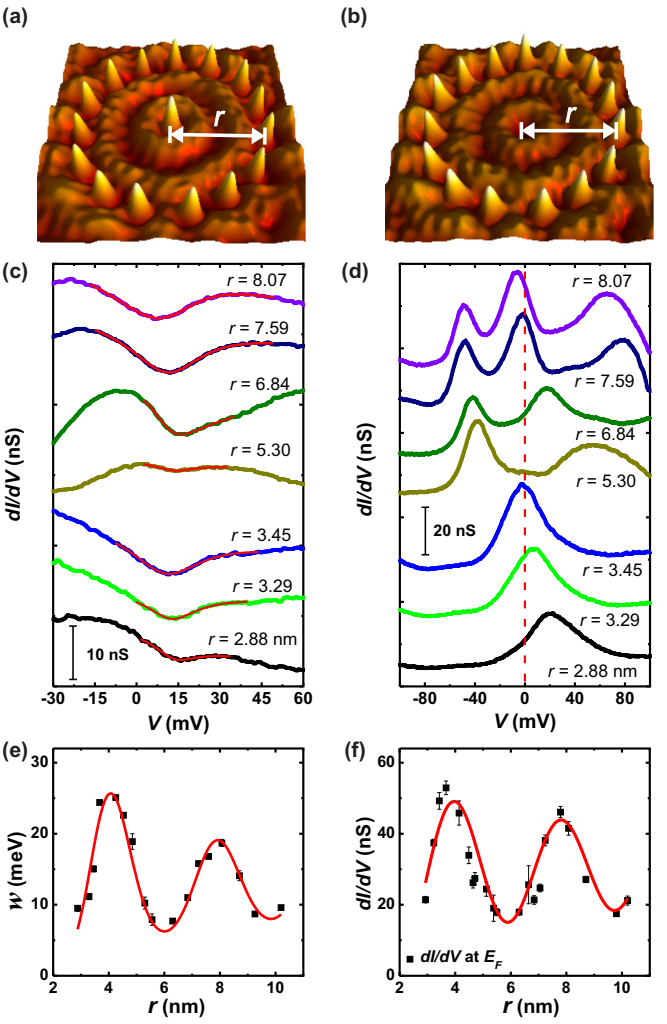

FIG. 4. (a) and (b) are topographic views of Co-centered and empty quantum corrals with the radius of r. (c) Representative dI/dV spectra on top of the Co adatom located at the center of the corral. (d) Representative dI/dV spectra at the center of empty corrals, $V_{\rm mod} = 4$ mV. (e) r-dependent Kondo resonance width. (f) r-dependent dI/dV at E_F obtained from (d). Red curves in (c), (e), and (f) are fittings (see text). In all measurements, $V_b = 50$ mV and $I = 1$ nA.

To make quantitative comparison, we performed fittings with Eqs. (3) and (4) for twin-atom and quantum-corral cases, respectively. The procedure is identical to the one applied for the step-edge case. We found that the fittings (red curves in Figs. 3 and 4) reproduce the experimental data in both cases. The results of dI/dV spectra fitting are listed in Table SI [38]. The extracted values J_b, J_s, δ_2, and $\tilde{D}$ are summarized in Table I. Remarkably, these values are almost the same correspondingly within experimental error for all three cases. This demonstrates the validity of the analytical method we used to analyze the Kondo effect in the presence of both bulk and surface states. By averaging them, we obtained $J_b = 0.51 \pm 0.04$ eV and $J_s = 0.26 \pm 0.05$ eV for the exchange constants between the Co adatom with the Ag(111) bulk and surface states. It is worth mentioning that the measured value $J_s = 0.26$ eV is comparable to the calculated value of 0.12 eV (see Supplemental Material [38]).

TABLE I. Exchange constants, phase shifts, and effective band cutoff obtained from the fittings.

	Twin atoms	Step edge	Quantum corral
J_b (eV)	0.55 ± 0.07	0.46 ± 0.05	0.53 ± 0.02
J_s (eV)	0.24 ± 0.15	0.33 ± 0.10	0.21 ± 0.02
δ_2 (rad)	-0.33 ± 0.12	-0.25 ± 0.19	-0.24 ± 0.06
$\tilde{D}$ (eV)	4.11 ± 2.74	5.36 ± 1.42	4.48 ± 0.62

IV. SUMMARY

In summary, we demonstrate the role of the surface state on the Kondo effect with the finding of the strong Kondo resonance width oscillations in a Co single adatom on a Ag(111) system. The oscillations have a period of half the Fermi wavelength of the surface state and increasing amplitude when a Co monomer is placed next to another Co monomer, near a step edge, and quantum confined within nanocorrals. With the combined LDOS and Kondo resonance measurements, we extract the exchange constants of the Co adatom with the Ag(111) bulk and surface states as $J_b = 0.51 \pm 0.04$ eV and $J_s = 0.26 \pm 0.05$ eV. Our experiments show that the Kondo resonance width can be continuously and significantly (greater than three times) tuned by quantum confinement of the surface state. This provides a pathway to tailor the Kondo effect.

ACKNOWLEDGMENTS

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