

**Luo *et al.* Reply:** In their Comment, Kolf *et al.* [1], criticizing our work on the Fano resonance for Anderson impurity systems [2], based their argument on the assumption that the Green's function of the  $d$  electron has approximately a Lorentzian form around the Kondo energy [Eq. (1) in Ref. [1]]. However, that assumption is inconsistent with the numerical renormalization group (NRG) results [3], revealing an asymmetric line shape of the impurity quasiparticle peak for systems without particle-hole symmetry, especially in the mixed valence regime. The asymmetric line shape, resulting mainly from the interference between the Kondo resonance and the broadening impurity level [2], can strongly affect the low energy behavior of conduction electrons, in particular, the differential conductance measured in STM experiments, and should not be ignored.

In their Comment, Kolf *et al.* correctly pointed out that Eq. (8) in Ref. [2] overestimates the asymmetry of the impurity line shape in the mixed valence regime. However, the error in Eq. (8) was not caused by Eq. (4) in Ref. [2] which is rigorous. It can be derived using the equation of motion method without invoking Wick's theorem. The error is instead due to an oversimplification in our approximate expression for  $T_d(\omega)$ , Eq. (7) in Ref. [2], containing a Kondo resonance pole and a slowly varying background. The correct low energy form of  $T_d(\omega)$  should be [4]:

$$T_d(\omega) \approx \frac{ae^{i\delta}}{\omega - \varepsilon_K + i\Gamma_K} + t_{\text{incoh}}, \quad (1)$$

where  $e^{i\delta}$  is the phase factor that was missed in Ref. [2]. In the Kondo limit,  $\delta \sim 0$  and  $a \sim \Gamma_K/\pi\rho_{d,0}$ , the above equation reduces to Eq. (7), while in the mixed valence regime missing of the phase factor leads to an overestimation of the line shape asymmetry. Replacing Eq. (7) in Ref. [2] with the above equation, the rest of derivations in Ref. [2] are still valid. Therefore our main physical picture and conclusions made in Ref. [2] remain unchanged.

Using Eqs. (4–6) in Ref. [2] and Eq. (1) here, we have reanalyzed the experimental data of Ti/Au and Ti/Ag systems, assuming  $U \rightarrow \infty$  for simplicity. The fitting parameters are  $(n, \varepsilon_d, \Delta, \varepsilon_K, \Gamma_K, a, \delta, q_c) = (0.38, 2.3, 65.0, -1.9, 4.0, 28.2, 2.7, 2.0)$  for Ti/Au and  $(0.53, 13.4, 38.8, -1.4, 5.2, 144.9, 3.0, 1.8)$  for Ti/Ag ( $\varepsilon_F = 0$  and the unit of energy is meV). Figure 1 shows that the experimental data can be well described by these equations. However, after the inclusion of the phase factor,  $\rho_d(\omega)$  can no longer be expressed in the simplified form of a Fano resonance as given by Eq. (8) in Ref. [2]. The insets show  $\rho_d(\omega)$  are asymmetric, but now without unphysical dip structure, in qualitative agreement with the NRG results [3]. The values of the fitting parameters indicate that both Ti/Au and Ti/Ag systems are in the mixed valence regime, being consistent with the experimental analysis and our previous conclusion. Thus their criticism that our analysis “is con-

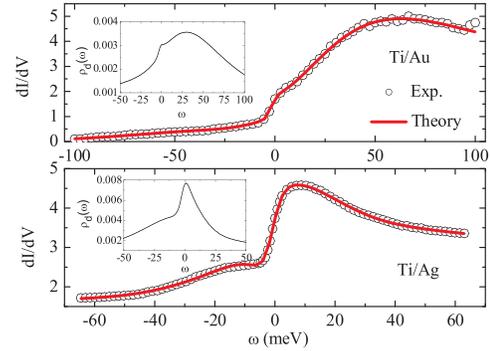


FIG. 1 (color online). Comparison between theoretical fitting curves and the STM experimental data for Ti/Au and Ti/Ag. The inset shows the corresponding impurity density of states.

ceptually incorrect and the quantitative agreement of . . . is meaningless” is unjustified.

The second comment of Ref. [1] is conceptually incorrect.  $\Delta$  and  $\Gamma_K$  result from two different physical effects and represent two different energy scales. They can certainly be distinguished, at least in the limit  $\Gamma_K \ll \Delta$  when the broadened impurity level can be taken effectively as a continuum channel and our theory can be applied. In the mixed valence regime, the fact that one cannot see a sharp peak with width  $\Gamma_K$  does not at all indicate the absence of that energy scale. In the third comment, the authors of Ref. [1] claimed that the values of  $\Delta$  we obtained for Ti/Au and Ti/Ag are too small. However, they did not give any firm evidence to support that claim. In fact, as revealed by experiments, the spectra for different transition metal atoms on Au surface behave very differently [5]. Thus, there is no reason to expect that the hybridization between a transition metal atom and conduction electrons should have the same order of magnitude.

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