Reply to Rodriguez and Goodman

On the basis of their commentary, we see that Rodriguez and Goodman have modified their initial position[1] that charge transfer between the metal adlayer and the substrate dominates the properties of bilayer systems. While we do not agree with everything in their comments on our article, there appears to be agreement on the following important points:

1. There are changes in the electron density of states of the adlayer due to rehybridization and other effects.
2. Charge transfer is small and does not account for the reduced metal CO reaction.
3. In the Pd/Ta case charge accumulates at the Pd/Ta interface.

We also think that everyone agrees that at least in the Pd/Ta case the core level shift of the adlayer is a result of the hybridized d band shift in the adlayer. Recent detailed theoretical work by Weinert and Watson[2] also confirms this. It is interesting that both the Commentary of Rodriguez and Goodman and our own work end in a similar way. They say, "The very good correlation found between the changes in the core levels of an admetal and variations in its ability to adsorb CO arises from the fact that both properties are very sensitive to perturbations in the valence d levels of the admetal."

We end our Account by saying, "We assert that a specific change in the overlayer valence electronic structure, namely, the change in the number of occupied and unoccupied states near the Fermi level, plays a crucial role in the bonding of CO to the surface and the dissociation of molecular hydrogen on the surface...".

In concluding, we think it is clear that valence band photoemission provides data that is essential for the understanding of the chemistry of transition metal overlayers on transition metal substrates. We thought we had shown this in studies[3] conducted in the early 1980s.

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(1) Rodriguez, J. A.; Goodman, D. W. *Science* **1992**, *257*, 897. See also the review by J. T. Yates: Yates, J. T. *Chem. Eng. News* **1992**, *70* (March 30), 22.

(2) Weinert, M.; Watson, R. E. *Phys. Rev. B*, in press.

(3) See, for example: El-Batanouny, M.; Strongin, M.; Williams, G. P.; Colbert, J. *Phys. Rev. Lett.* **1981**, *46*, 269. Ruckman, M. W.; Strongin, M. *Phys. Rev.* **1984**, *29*, 7105.

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