Juaristi *et al.* Reply: In the preceding Comment [1] on our recent Letter [2], Luntz *et al.* claim that their results show that the local density approximation for electronic friction (LDAF) is in general not reliable for estimating the electronic friction for molecules on metal surfaces. This is an unfounded statement based on very limited information.

Our LDAF calculation for the friction coefficient involves at most two further approximations as compared to those involved in the model used by Luntz *et al.*. (i) First, a local approximation for the electronic density is used. This is acknowledged to be a reasonable approximation. The LDAF was shown to be appropriate for calculations of the friction coefficient for atoms in metal surfaces, incidentally by some of the authors of the comment [3]. (ii) An additional approximation is that two-center effects are disregarded. Two-center effects were shown not to change the order of magnitude in the case of H_2 [4], but no studies in other systems have been performed to our knowledge. Therefore, it is plausible that two-center effects may affect in some cases the value of some components of the friction tensor, in particular, those associated to vibrations along the molecular axis (η_{dd}), as those shown by Luntz *et al.* in their figure for N_2/Ru(0001).

But let us emphasize that realistic theoretical studies on the dynamics of diatomic molecules on surfaces should be at least six dimensional. It is well known that simpler models based on lower dimensions lead to erroneous conclusions in many systems and, in particular, for N_2/Ru(0001) that is precisely one of the systems used by the authors of the Comment (see for instance the discussion in Ref. [5]). In their low-dimensional analysis, Luntz *et al.* are comparing just a small portion of the friction tensor (2 components out of a 6×6 tensor), over a small and *arbitrary* region of the multidimensional potential energy surface. The fact that this path represents the minimum energy path in two dimensions (with the arbitrary *constraint* that the molecule stays oriented parallel to the surface) is not necessarily relevant in a fully six-dimensional dynamics. Therefore, although the particular discrepancy shown by Luntz *et al.* for N_2 in Ru(0001) clearly requires further methodological investigation, it cannot be used as grounds for a general claim.

On the contrary, the comparison of our six-dimensional theoretical calculation including friction with experimental results suggests that the order of magnitude of the LDAF friction coefficients in the case of N_2/W(110) and H_2/Cu(110) is correct in the regions of the potential energy surface important for the dynamics [2,6,7], though discrepancies in some particular cases may exist. Therefore, we go on claiming that the contribution of electron excitations to the dissociative sticking of N_2 in W(110) and H_2 in Cu (110) is a marginal correction and that an adiabatic calculation is still meaningful.

J. I. Juaristi,[1,2,3] M. Alducin,[2,3] R. Díez Muiño,[2,3] H. F. Busnengo,[4] and A. Salin[3]
[1]Departamento de Física de Materiales
Facultad de Químicas
UPV/EHU
Apartado 1072, 20080 San Sebastián, Spain
[2]Centro de Física de Materiales Centro Mixto CSIC-UPV/EHU
Edificio Kort,
Avenida de Tolosa 72, 20018 San Sebastián, Spain
[3]Donostia International Physics Center DIPC
Paseo Manuel de Lardizabal 4, 20018 San Sebastián, Spain
[4]Instituto de Física Rosario (CONICET-UNR)
and Facultad de Ciencias Exactas, Ingeniería y Agrimensura
Universidad Nacional de Rosario
Avenida Pellegrini 250, 2000 Rosario, Argentina

Received 26 January 2009; published 10 March 2009
DOI: 10.1103/PhysRevLett.102.109602
PACS numbers: 82.65.+r, 34.35.+a, 68.49.Df, 82.20.Kh

[1] A. C. Luntz *et al.*, preceding Comment, Phys. Rev. Lett. **102**, 109601 (2009).
[2] J. I. Juaristi, M. Alducin, R. Díez Muiño, H. F. Busnengo, and A. Salin, Phys. Rev. Lett. **100**, 116102 (2008).
[3] M. Persson and B. Hellsing, Phys. Rev. Lett. **49**, 662 (1982).
[4] R. Díez Muiño and A. Salin, Phys. Rev. B **62**, 5207 (2000).
[5] C. Díaz *et al.*, Phys. Rev. Lett. **96**, 096102 (2006).
[6] M. Alducin, R. Díez Muiño, H. F. Busnengo, and A. Salin, Phys. Rev. Lett. **97**, 056102 (2006).
[7] A. Salin, J. Chem. Phys. **124**, 104704 (2006).

