

**Erratum: Six-Dimensional Quantum Dynamics of Dissociative Chemisorption
of ($\nu = 0, j = 0$) H_2 on Cu(100)
[Phys. Rev. Lett. 78, 3583 (1997)]**

G. J. Kroes, E. J. Baerends, and R. C. Mowrey

[S0031-9007(98)07822-3]

The six-dimensional potential V_{6D} [1] that was used in the quantum dynamics calculations on $H_2 + Cu(100)$ contained an artificial well in the entrance channel, the depth of the well being 0.19 eV. This well occurred for impact on the bridge site, $\theta = 90^\circ$, and ϕ such that the atoms move to top sites, for a molecule-surface distance $Z \approx 7a_0$ and H-H distance $r \approx 1.4a_0$. The well was due to erroneous extrapolation. The function V_{3b}^A that was employed in the fit [Eq. (6a) of Ref. [1]] did not go to zero fast enough with increasing Z .

The problem of V_{3b}^A not being well behaved at large Z can be avoided by switching of the molecule-surface interaction at a point where it has become small enough to do so without introducing large errors. Consequently, we have changed the parameters of $f_c(Z)$ [Eq. (2) on p. 3583] to switch off the interaction between 5 and 5.8 bohr, instead of between $8.14a_0$ and $8.94a_0$ as done originally. (Note that the fit is based on electronic structure calculations performed for Z up to $5a_0$. Also note that a procedure in which V_{3b}^A is switched off only for bridge-to-top dissociation [1] also works well [2] but is less general.)

The 6D results obtained using the improved potential for the dissociation and vibrational excitation of ($\nu = 0, j = 0$) H_2 are shown in Fig. 1. A corrected version of Table I (p. 3585) is also given. As evidenced by Table II, the use of the corrected potential has led to a substantial improvement in the agreement between theory and experiment [3]. The new values for the saturation parameter A and the dynamical threshold E_0 [see Eq. (1), p. 3583] are in much better agreement with the fit to experiments than before. In particular, the calculated dynamical threshold E_0 is now too high by 0.1 eV, rather than 0.18 eV. The new results suggest that the barriers in the potential are too high on average by ≈ 0.1 eV. This result is subject to uncertainties as previously discussed. Our previous conclusions, that vibrational excitation on Cu(100) is substantial at large energies (Fig. 1) and that the motion in all six degrees of freedom of H_2 needs to be taken into account (Fig. 2, p. 3585), remain unaffected.

We are grateful to Drew McCormack for bringing the error to our attention.

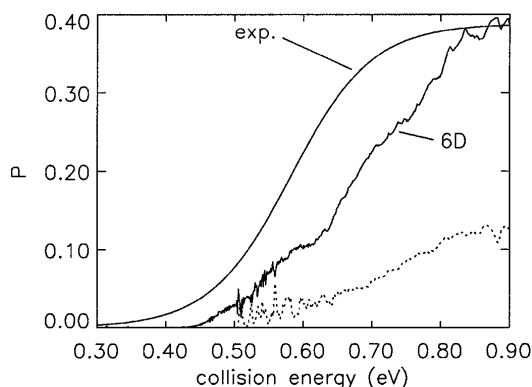


FIG. 1. The 6D probability for dissociation is compared to the experimental reaction probability curve [3]. Also shown is the calculated probability for vibrational excitation $P(\nu = 0 \rightarrow 1)$ (dotted curve).

TABLE I. Reaction probabilities R_0 and probabilities for vibrational excitation $P(\nu = 0 \rightarrow 1)$ are given for a few collision energies E_i .

E_i (eV)	R_0	$P(\nu = 0 \rightarrow 1)$
0.45	0.004	0.0
0.55	0.072	0.006
0.65	0.153	0.046
0.75	0.266	0.084
0.85	0.370	0.122

TABLE II. The experimental ("expt") values of A and E_0 are compared to the new (new T) and the old (old T) theoretical results.

Parameter	Expt	New T	Old T
A	0.388	0.39	0.28
E_0 (eV)	0.582	0.68	0.76

[1] G. Wiesenekker, G. J. Kroes, and E. J. Baerends, *J. Chem. Phys.* **104**, 7344 (1996).

[2] D. A. McCormack, G. J. Kroes, E. J. Baerends, and R. C. Mowrey, *Faraday Discuss.* (to be published).

[3] H. A. Michelsen and D. J. Auerbach, *J. Chem. Phys.* **94**, 7502 (1991).