Erratum

Erratum to ''Different adsorbate binding mechanisms of hydrocarbons: Theoretical studies for Cu(111)–C_2H_2 and Cu(111)–C_2H_4'' [Applied Catalysis A: General 172 (1998) 85–95]*

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The publisher regrets the poor quality reproduction of Figs. 1–3 in the above article. These figures are re-printed overleaf.

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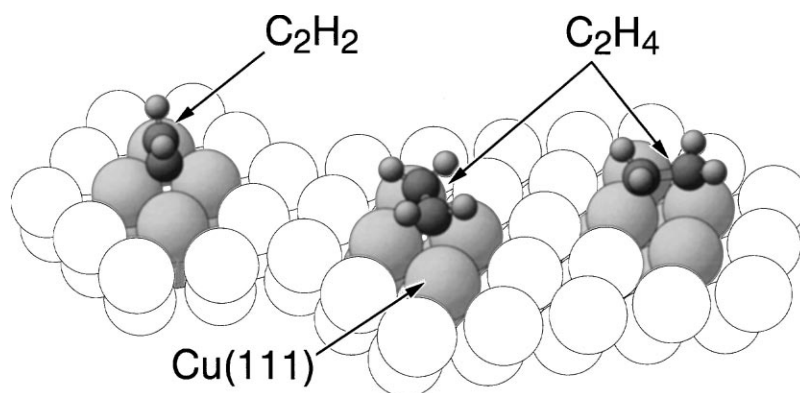* PII of original article S0926-860X(98)00108-2

Fig. 1. Geometric structure of the $Cu_7(4,3)C_2H_2$ and $Cu_7(4,3)C_2H_4$ clusters used in the present study. The left part of the figure shows the cross-bridge orientation of the C_2H_2 adsorbate. For adsorbing C_2H_4, two surface orientations are considered: (middle) cross-bridge, and (right) di-σ. The light balls in the figure represent Cu substrate atoms (not included in the clusters) which are meant to illustrate the Cu(111) surface geometry.
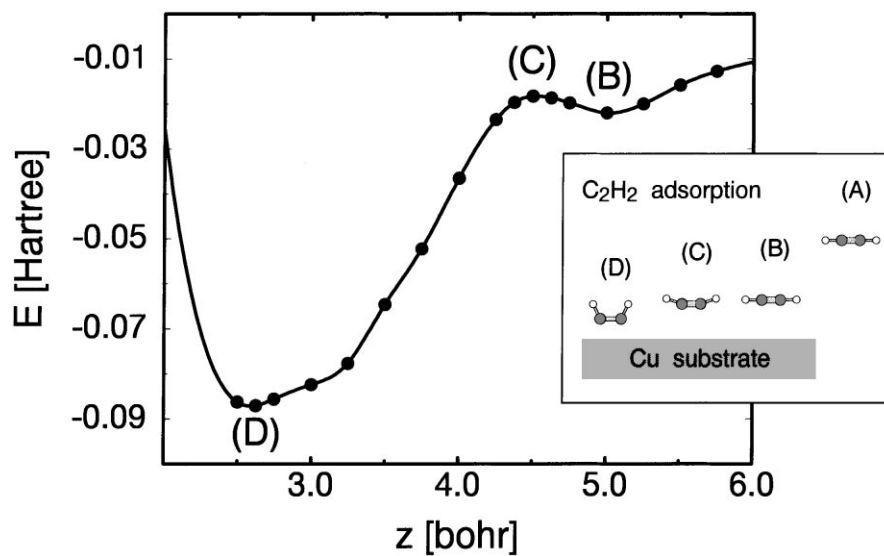

Fig. 2. Total energy curve $E(z)$ for the $Cu_7(4,3)C_2H_2$ cluster along an adiabatic adsorption path obtained from a restricted optimization (see text). The inset visualizes the geometry of the adsorbate at four selected points of the path: (A) free C_2H_2 molecule, (B) outer minimum, (C) barrier, and (D) inner minimum.
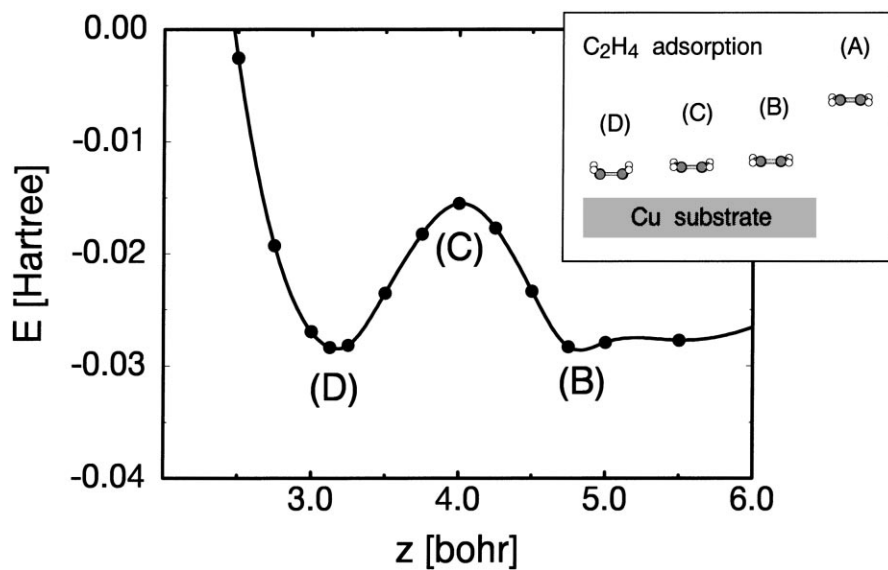
Fig. 3. Total energy curve $E(z)$ for the $Cu_7(4,3)C_2H_4$ cluster along an adiabatic adsorption path obtained from a restricted optimization with the C_2H_4 in cross-bridge orientation (see text). The inset visualizes the geometry of the adsorbate at four selected points of the path: (A) free C_2H_4 molecule, (B) outer minimum, (C) barrier, and (D) inner minimum.