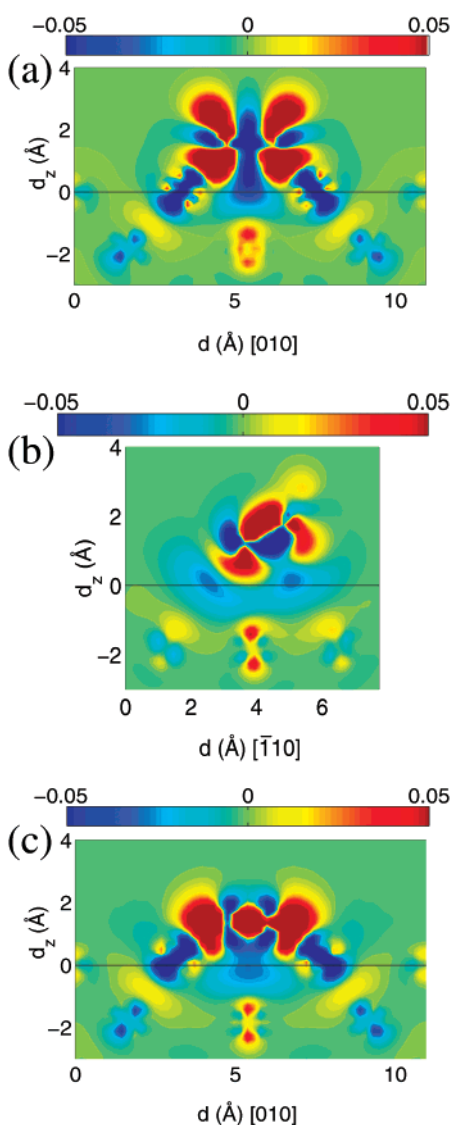


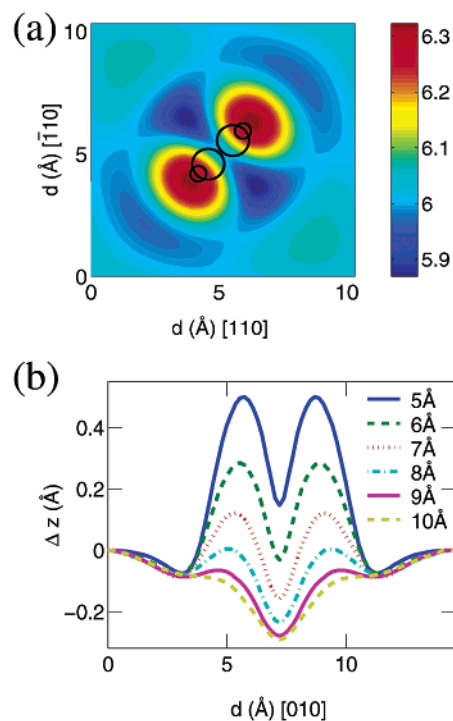
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F. E. Olsson, M. Persson,\* N. Lorente, L. J. Lauhon, and W. Ho: STM Images and Chemisorption Bond Parameters of Acetylene, Ethynyl, and Dicarbon Chemisorbed on Copper

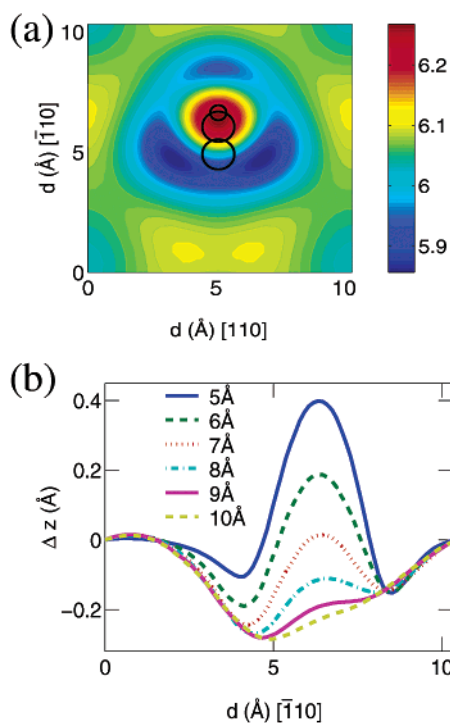
Pages 8161–8171. The authors show here color representations of Figures 7, 9, 10, 11. This paper was originally published as part of the special issue “John C. Tully Festschrift”.



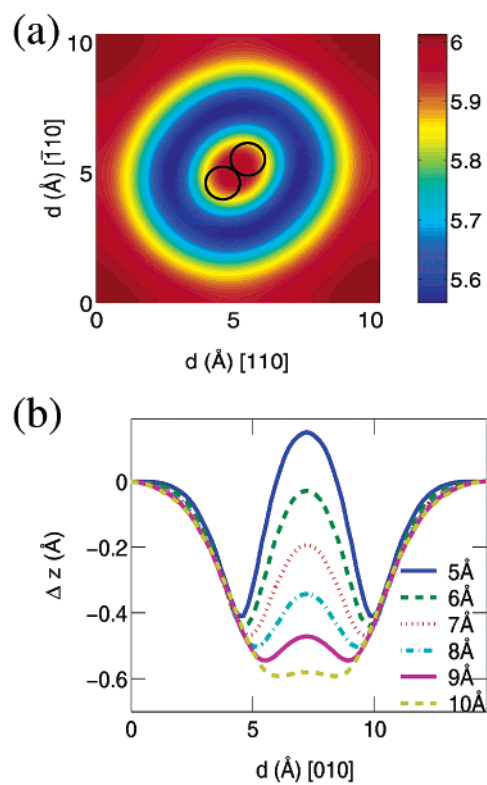
**Figure 7.** Density difference contours along the C–C axes of (a)  $C_2H_2$ , (b)  $C_2H$ , and (c)  $C_2$ . Density differences for values larger than 0.05 and less than  $-0.05$  electrons/ $\text{\AA}^3$  are truncated.  $d_z = 0$  corresponds the position of the surface layer. The calculation has been carried out in a  $3 \times 3$  surface unit cell with 16  $k$  points in the SBZ.



**Figure 9.** Calculated LDOS (a) image and (b) profiles along the C–C axis for  $C_2H_2$  chemisorbed on Cu(001), where  $\Delta z = 0$  corresponds to tip–surface distances of  $z_0 = 5, 6, 7, 8, 9,$  and  $10$  Å, (a)  $z_0 = 6$  Å. The geometric configuration of the chemisorbed  $C_2H_2$  is indicated in the LDOS image. The calculation was carried out using a  $4 \times 4$  surface unit cell with 16 points in the SBZ and Gaussian broadening of  $\sigma = 0.25$  eV.<sup>21</sup>



**Figure 10.** Calculated LDOS (a) image and (b) profiles along the C–C axis for C<sub>2</sub>H chemisorbed on Cu(001), where  $\Delta z = 0$  corresponds to tip–surface distances of  $z_0 = 5, 6, 7, 8, 9,$  and  $10 \text{\AA}$ , (a)  $z_0 = 6 \text{\AA}$ . The geometric configuration of the chemisorbed C<sub>2</sub>H is indicated in the LDOS image. Same surface unit cell,  $k$ -point set, and  $\sigma$  as in Figure 9.



**Figure 11.** Calculated LDOS (a) image and (b) profiles along the C–C axis for C<sub>2</sub> chemisorbed on Cu(001), where  $\Delta z = 0$  corresponds to tip–surface distances of  $z_0 = 5, 6, 7, 8, 9,$  and  $10 \text{\AA}$ , (a)  $z_0 = 6 \text{\AA}$ . The geometric configuration of the chemisorbed C<sub>2</sub> is indicated in the LDOS image. Same surface unit cell,  $k$ -point set, and  $\sigma$  as in Figure 9.

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