


Fig. 2 (a)-(e) $2\sigma_g$, $2\sigma_u$, $3\sigma_g$, $1\pi_u$, $1\pi_g$. The upper contour plots refer to the pseudopotential change densities, the lower plots to the all electron results of Ref. 9. The arrows point to the contours which approximately correspond to each other in space. The contour value associated to one electron in the superlattice unit cell is given for comparison. The smallest contour value of each plot is equal to the contour separation. The black dots indicate the position of the nuclei. (f) Total charge contour plots. Conventions as before.

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