

COMMENT

**Comment on ‘Surface reconstruction on Si(100) studied by the CNDO method’**

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In a recent paper Ong and Chan [1] examined seven different asymmetric dimer reconstructions for a Si(100) surface using the CNDO (complete neglect of differential overlap) method. The  $p(4 \times 1)$  and  $c(4 \times 2)$  reconstructions were found to be energetically more favourable, followed by  $p(2 \times 2)$  and  $(2 \times 1)$ . In this comment I will discuss only the results of the four members of the  $(2 \times 1)$  family, since experimentally the other asymmetric dimer reconstructions are not observed on the Si(100) [2] and the Ge(100) [3] surfaces. Ong and Chan [1] made a cluster calculation with only eight Si atoms in the first layer, resulting in four dimers for the  $(2 \times 1)$  family. Their results for the total energy per dimer for the members of the  $(2 \times 1)$  family are summarised in the first column of table 1.

As to these structures, I have calculated the electrostatic energy contribution to the total energy per dimer ( $\Delta$ ) of all the other dimers outside the cluster (see second column of table 1). For the charge transfer ( $0.14e$ ), the dimer length ( $2.38 \text{ \AA}$ ) and the dimer tilt ( $14^\circ$ ) the values of Ong and Chan [1] have been taken, of course. This proves that, taking into account the electrostatic energy contribution of the dimers outside the cluster, the  $c(4 \times 2)$  and  $p(2 \times 2)$  asymmetric dimer reconstructions become lowest in energy [4], in agreement with low temperature experiments at the Si(100) [2] and Ge(100) [5, 6] surfaces. The  $p(4 \times 1)$  asymmetric dimer reconstruction, which is never observed experimentally, is now found to be energetically unfavourable compared with the  $c(4 \times 2)$  and  $p(2 \times 2)$  reconstructions (see third column of table 1).

**Table 1.** Results of the total energy/dimer for the four members of the  $(2 \times 1)$  family.

Reconstruction	eV/dimer Si(100) [1]	eV/dimer $\Delta$	eV/dimer adjusted results
$(2 \times 1)$	-1.21	0.0013	-1.21
$p(2 \times 2)$ or $2 \times 2A$	-1.22	-0.011	-1.23
$p(4 \times 1)$ or $4 \times 1$	-1.27	0.048	-1.22
$c(4 \times 2)$ or $4 \times 2$	-1.27	-0.012	-1.28

In conclusion, one has to be careful in drawing conclusions from small cluster calculations with respect to the energy differences for asymmetric dimer reconstructions. Taking into account the electrostatic interaction with dimers outside the cluster can alter the results significantly.

## References

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