

## E1-30 Oxygen stabilization of the (1x1) Pt (001) surface

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Pt(001) is characterized by surface reconstruction. The (5x20) reconstruction is inhibited in the (1x1) phase with sufficient oxygen coverage. In this study, the surface embedded Green function (SEGF) method has been used to perform self-consistent calculations of the surface electronic structures of (1x1)Pt(001) and p(1x1) oxygen on Pt(001). It shows a reduction of surface stress upon oxygen chemisorption.

In the SEGF method, the semi-infinite crystal is divided into 2 regions: the surface (a slab consisting of a few atomic layers) and the bulk substrate. The effect of the substrate on the surface wave function is included through an embedding potential, which is the inverse of the Green function for the bulk.

The surface charge density can be used to calculate the bond order for the surface atoms. If  $F_2$  is the attractive bonding force of sp electrons in the bulk, the net compressive force

$$\text{per bond at the surface is } F = \frac{B_s}{B_b} - 1 F_s$$

Where,  $B_s$  and  $B_b$  are the bond order for the surface and the bulk. For O/Pt system the surface region consists of one layer each of oxygen and platinum atoms.

The mid-bond sp charge densities of clean Pt(001) and oxygen covered platinum were calculated as  $0.023 \text{ \AA}^{-3}$  and  $0.019 \text{ \AA}^{-3}$ . Therefore,  $B_s$  for the (1x1)Pt(001) surface and the oxygen covered surface are 0.68 and 0.37 and  $B_b$  is 0.45. The calculated surface stresses (compressive) for the (1x1)Pt(001) and O/Pt(001) are  $-0.12 \text{ eV \AA}^{-2}$  and  $-0.04 \text{ eV \AA}^{-2}$ , respectively. The reduction of the surface stress shows the stability of the (1x1)Pt(001) surface in the presence of oxygen.