# Silicon oxidation suppressed by electron overresponse to O adsorption on Sr-covered Si(001)

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An intriguing route to transferring electronics to spintronics is to integrate oxides on a Si substrate. The pre-growth of Sr layer was also found to be able to protect the underlying silicon and form a sharp interface between Si and oxides(STO). Based on first principles calculations, we reveal the role of the pre-growth Sr layer in blocking silicon oxidation during the initial growth of $SrTiO_3$ on Si(001). It is found that the Sr-covered Si(001) behaves distinctively different to the clean Si(001) in response to O adsorption: through redimerization of Si atoms beneath the Sr layer, the Sr-covered Si(001) behaves as an electron-reservoir and releases more electrons than that required to saturate O. Widely distributing and easily moving on the surface, these excess electrons in overresponse to the O adsorption increase the barrier of O into the Sr layer to form silicon oxidation, giving rise to a high quality interface between $SrTiO_3$ and Si(001).

## 1. *Electron over-response* of full Sr monolayer covered Si(001) for O adsorption

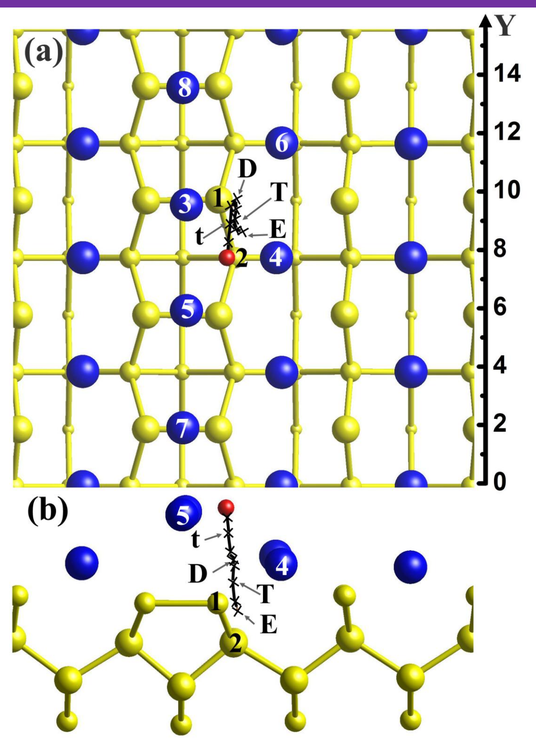


Fig.1 Topview (a) and sideview (b) of the most stable configuration for a single O atom adsorption on a Sr-covered Si(001). The yellow, blue and red balls represent Si, Sr and O atoms, respectively. The crosses indicate the O's positions of the CNEB images along the pathway from the initial state to the oxidized Si-backbond state on the Sr-covered Si(001), and the sold line links the crosses as an eye guide.

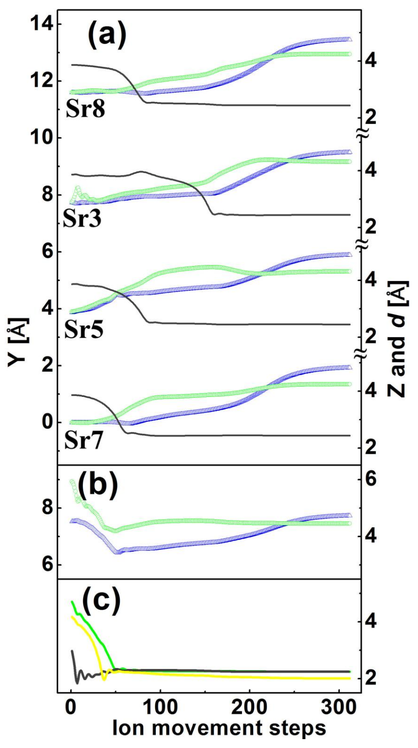


Fig.2 Trajectories of the concerned atoms and variations of the bond lengths for four pairs of surface Si atoms during the adsorption process. The blue (dark) and green (light) dots are the trajectories of *y* and *z*-coordination of Sr atoms relative to ion movement steps. The trajectory of O is plotted in figure (b), and the blue (dark) and green (light) dots indicate also its *y* and *z*-coordination , respectively. In figure (c) the green, yellow and black lines for the distance of O to $Sr_3$, $Sr_4$ and $Sr_5$ , respectively.

## 2. Physics behind over-response

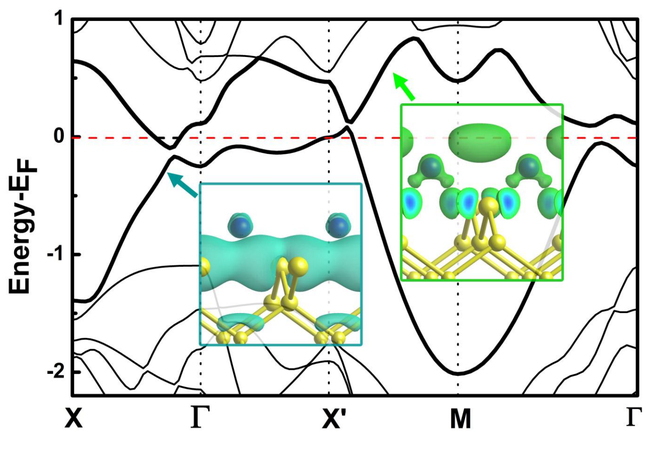


Fig.3 Nearly full occupied dangling bond and nearly full empty Sr's orbit on Sr covered Si(001) 1X1 surface

## 3. *Barrier enhancement and energy inversion* in oxidation process of Sr covered Si(001)

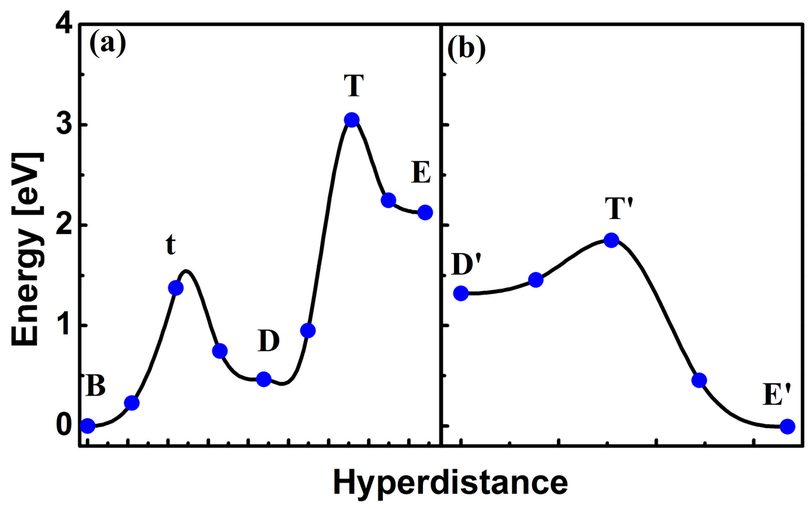


Fig.4 Energy variation along the reaction pathway between the initial state of O adsorption and the state of oxidized Si-backbond on Si(001) with (a) and without (b) Sr covering.

## 4. Role of Sr in the silicon oxidation process

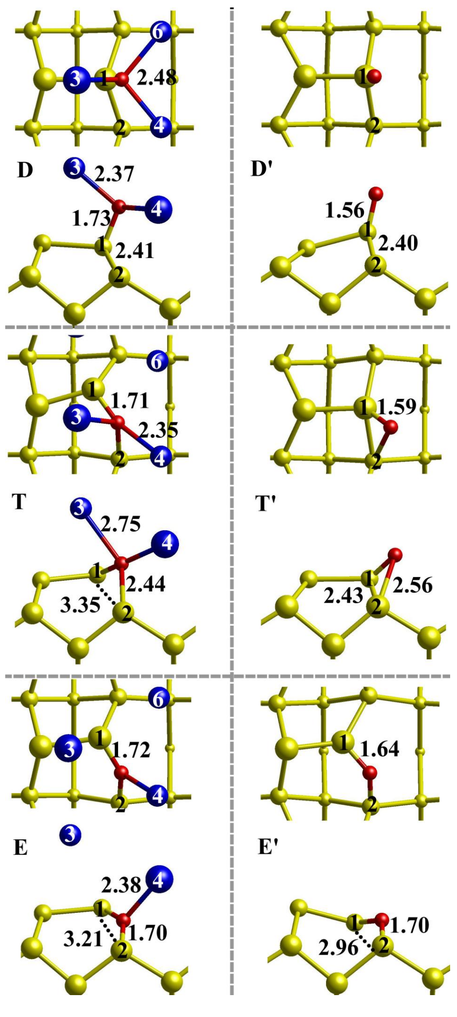


Fig 5 The same as Fig. 1, but for states D (D'), T (T') and E (E') with (without) Sr covering. The bond lengths are indicated in angstroms.

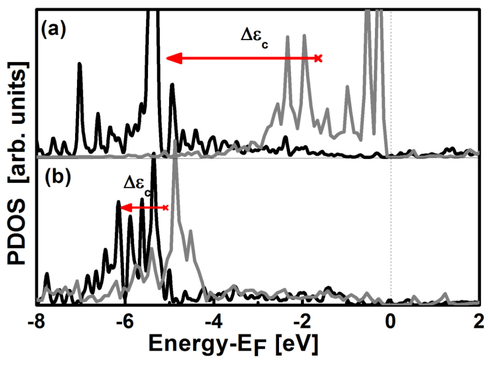


Fig.6 Projected density of state (PDOS) of O's p-orbitals for states D and D' (a), E and E' (b). The black and gray lines present PDOS on Si(001) with and without Sr covering, respectively. Shifts of the occupied band center of these orbitals are indicated by arrows.