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## First-principles study of the initial-stage oxidation of Si(111)-(7x7)

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Chemisorption of oxygen molecules on the Si(111)-(7x7) surface has been studied extensively as a model for the initial-stage oxidation of the surface. The basic step to the surface oxidation is the dissociation of the adsorbed O<sub>2</sub> molecules, but the dissociation procedure and the atomic structure of the reaction products still remains as a subject of debates.

We present here density-functional theory calculations on the initial-stage oxidation states of the Si adatom site for all possible dissociation configurations that can be generated by multiple O<sub>2</sub> reactions. We determine the equilibrium structures and analyze their electronic and vibrational properties in comparison with measured UPS, XPS, and EELS spectra.

The O(ad) atom bonded on top of the Si adatom is always less stable than the O(ins) atom inserted into one of the adatom backbonds. Our electronic and vibrational analysis demonstrates further that the O(ad) and O(ins) atoms account well for the metastable and stable features in previous experiments, respectively. Moreover, the calculated decay pathways of the metastable structures and the comparison of the calculated O 1s core-level shifts with XPS data provides a convincing argument in unambiguously identifying the experimental metastable and stable structures, thereby making it possible to build a correct atomic-scale picture of the initial-stage oxidation process on this surface.