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First-principles calculations that clarify energetics and reactions of oxygen adsorption and carbon desorption on 4H-SiC (11-20) surface HAN LI, YU-ICHIRO MATSUSHITA, The University of Tokyo, MAURO BOERO, IPCMS, ATSUSHI OSHIYAMA, The University of Tokyo — Silicon carbide(SiC) is a well-known and now an emerging semiconductor material for power electronics due to its wide band-gap and the robustness under harsh environment. Oxidation of SiC leads to the formation of SiO_2 on the semiconductor surface which is essential in the transistor action of the devices, as in the case of Si. However, the formation of the SiO_2 films on the compound semiconductor SiC is much more complicated phenomenon since oxygen reacts with both Si and C, and then C atoms are eventually annihilated. We report static and dynamical first-principles calculation that provide atomistic pictures at the initial stage of the oxidation of the (11-20) surface of 4H-SiC. The oxygen adsorption shows structural multi-stability and the surface bridge sites are the most stable. An arriving O_2 molecule is adsorbed, dissociated and then migrates toward these surface bridge sites with the free-energy barrier of 0.7 eV. We also find that a CO molecule is desorbed from the metastable oxidized structure with the free-energy barrier of about 2.5 eV. Drastic reduction of the CO desorption energy is found on the (000-1) surface and the reason is clarified to be the electron transfer from the Si to C dangling bonds.

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