First-principles investigation of the mechanism of oxidation in atomic layered MoS_2 structures

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Abstract

Two-dimensional transition metal dichalcogenides (TMDCs) has attracted a great deal of attention due to its unique properties. For electronic and optoelectronic device applications of TMDCs, the oxidation mechanisms studies are important. Herein, we investigate the oxidation mechanisms of MoS_2 layer carrying out density functional theory (DFT) calculations. We analyze the atomic and electronic properties of oxidized MoS_2 layer structures. We find that the first step of the oxidation process occurs at the edge and top basal plane of MoS_2. The MoS_2 nanocluster has a bending structure after fully oxidation of top basal plane. We suggest that the bending and opening of edges is the key step that allows the self-limiting layer-by-layer oxidation of multilayer MoS_2. The opened edge atomic structures of MoS_2 nanocluster make enough space to insert the oxygen atom at the interface of bilayer MoS_2. We will also consider the diffusion pathway of oxygen atoms into interface and calculate the stable structures of oxidation on the two sides of bilayer MoS_2. The accumulated understanding of oxidation mechanisms can be applied to achieve the refined control of TMDCs oxidation processes, which will allow the synthesis of atomically precise MoS_2-MoO_3 heterostructures and the prevention of MoS_2 oxidation under ambient and oxidative conditions. Based on these result, we provides the basic understanding on the oxidation mechanism of TMDCs materials.

References

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Figures

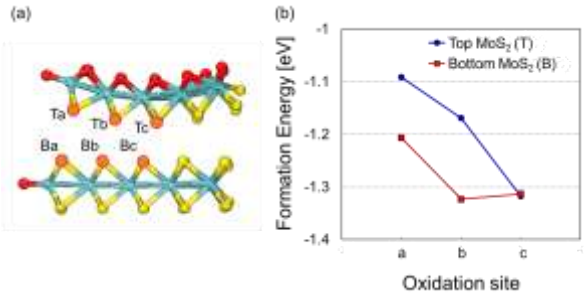

Figure 1: (a) An atomistic model of the oxidized zigzag MoS_2 nanoribbon (b) Oxidation energies of a, b, and c sites for T and B.