Adsorption of Gas Molecules on the LaB_6(100) Surface: A DFT Study

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Lanthanum hexaboride (LaB_6) boasts exceptional properties, such as, a low work function [1-3], excellent chemical inertness [4], low evaporation rate and nearly equivalent evaporation rates for both lanthanum (La) and boron (B) [5]. The thermal electron emission process remains stable in a vacuum environment [6]. These outstanding properties of lanthanum hexaboride render it an ideal material for the fabrication of field emission scanning electron microscope (FE-SEM) cathodes. Although tungsten is more commonly used as a cathode material, lanthanum hexaboride, with its lower work function, is regarded as a superior electron emission material with significant potential for diverse applications. By the 1960s and 1970s, significant researches had been conducted on the field emission properties of lanthanum hexaboride [7-9]. However, residual gas molecules in a vacuum can poison lanthanum hexaboride, leading to a reduced emission current density. Previous studies on the poisoning mechanism of lanthanum hexaboride have shown that nitrogen or oxygen in residual gases reduces emission current density [10].

In this work we have calculated the adsorption of several common gas molecules on the LaB_6(100) surface. For the adsorption of each gas molecule, we have selected the most stable molecular adsorption and dissociative adsorption structures based on the adsorption energy, as shown by Fig. 1 for CO_2 on the LaB_6(100) surface. We calculated the work function of all stable adsorption structures, and the results show that for the most stable adsorption structure, the adsorption of gas molecules will lead to an increase in the work function of the LaB_6(100) surface, which will reduce the probability of electron tunneling and thus decrease the cathode current, leading to poisoning of the LaB_6 cathode. Subsequently, we calculated the charge transfer, and for all the stable adsorption structures, a transfer of electrons from the LaB_6(100) surface to the gas molecules was found. This charge transfer will produce a dipole moment on the surface, and the appearance of this dipole moment is the reason for the increase in surface work function. Moreover, the dissociative adsorption of the same molecule always involves more electron transfer than molecular adsorption. To further investigate the charge transfer, we also calculated the differential charge density to visualize the charge transfer; the differential charge density can help us further analyze the bonding of the adsorbed molecules with the surface. In addition, we have have performed DOS calculations for all the stable molecular structures to further analyze the bonding situation on the surface.

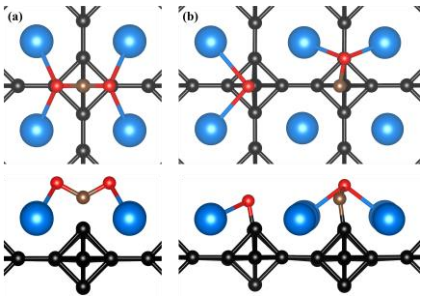

Figure 1. The most stable configurations of CO_2 on the LaB_6(100) surface: (a) molecular adsorption; (b) dissociative adsorption.

Keywords: lanthanum hexaboride; gas adsorption; density functional theory; charge transfer.

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BIOGRAPHY

Rui Wang has completed his bachelor degree in 2021 from Hefei University of Technology and now is a master student at University of Science and Technology of Chia. His main research direction is DFT.