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Lattice relaxation as the origin of the insulating nature of the alkali/Si(111):B surface LAURENT CHAPUT, CEDRIC TOURNIER-COLLETTA, LOUIS CARDENAS, BERTRAND KIERREN, YANNICK FAGOT-REVURAT, DANIEL MALTERRE, Institut Jean Lamour, PATRICK LEFEVRE, FRANCOIS BERTRAN, synchrotron soleil, ANTONIO TEJEDA, Institut Jean Lamour, AMINA TALEB, synchrotron soleil — *Ab initio* density-functional theory calculations, photoemission spectroscopy (PES), scanning tunneling microscopy, and spectroscopy (STM, STS) have been used to solve the $2\sqrt{3} \times 2\sqrt{3}R30$ surface reconstruction observed previously by LEED on 0.5 ML K/Si:B. It is found that the large K-induced vertical lattice relaxation obtain in the calculations and occurring only for 3/4 of Si adatoms is shown to quantitatively explain both the chemical shift of 1.14 eV and the ratio 1/3 measured on the two distinct B 1s core levels. A gap is observed between valence and conduction surface bands by ARPES and STS which is shown to have mainly a Si-B character using the ab initio calculations. Finally, the calculated STM images agree with our experimental results. Therefore, the insulating character of alkali/Si:B interfaces has been captured to an excellent accuracy, from the low lying 1s state of boron, to the unoccupied states above the gap, within a one-electron approach. This work solves the controversy about the origin of the insulating ground state of alkali-metal/Si(111):B semiconducting interfaces which were believed previously to be related to many-body effects

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