P10 DFT-D study of the cycloaddition reaction on boron doped silicon surfaces

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ABSTRACT

In this work, we have investigated the molecule adsorption on Si(111)√3x√3R30°-B (denoted by SiB) surfaces within the Density Functional Theory (DFT- D) method [1]. The SiB substrate is considered in three cases: defectless SiB surface (denoted SiB-0D) and SiB surfaces presenting one or two boron defects (denoted SiB-1D and SiB-2D respectively).

The SiB-0D surface is passivated by a charge transfer from the Si adatoms to the boron atoms and therefore no chemical bond between the molecule and the substrate is observed.

In the SiB-2D case, a similar molecular adsorption as already evidenced in the HPc–SiC(0001)3x3 system is involved [2,3].

In the case of the SiB-1D surface, two Si–N bonds (denoted Si1–N1 and Si2–N2) are observed. One of them, Si1–N1, is nearly similar to that found in the HPc–SiB-2D system, but the Si2–N2 bond is unexpected. The Bader charge analysis suggests that, in the presence of the Hc molecule, the boron atoms behave like an electron reservoir whose availability varies following the involved molecular adsorption process. In the SiB-1D case, charges are transferred from the substrate to the molecule, allowing the Si2–N2 bond formation. Such a kind of molecular adsorption, not yet observed, could be designed by ''assisted pseudo-cycloaddition''.

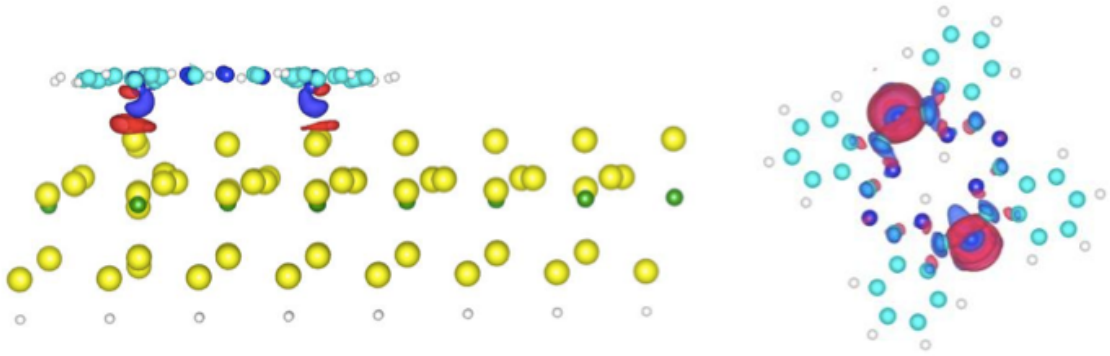

Fig. 1 : Side and top views of the charge density difference of the H adsorption on the SiB-1D surface. In order to facilitate the interpretation, the atoms of the substrate are removed in the top view. Blue and red plots correspond to positive and negative electronic charge variations respectively. Yellow, green, light blue, dark blue and white circles correspond to silicon, boron, carbon, nitrogen and hydrogen atoms respectively.

REFERENCES

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