

## P9 Molecular chemisorption on boron doped silicon surfaces: DFT study

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### ABSTRACT

By means of density functional theory calculations, we have investigated the adsorption of a single trans 4-pyridylazobenzene molecule (denoted by PAB) on doped boron Si(111) $\sqrt{3}\times\sqrt{3}$ R30° surface (denoted by SiB) with or without boron-defect [1]. The dispersion corrections have taken into account within the approach proposed by Grimme. Two adsorption configurations are electronically studied. In the first one, the molecule is parallel to the surface and interacts with the SiB surface via the -N=N- bond. In presence of a boron-defect, a Si-N chemical bond between the molecule and the surface is then formed, while electrostatic or/and van der Waals interactions are observed in the defectless surface.

In the second adsorption configuration, the molecule presents different orientations with respect to the surface and interacts via the nitrogen atom of the pyridyl part of the PAB molecule. If the molecule is perpendicular to the perfect SiB surface, the lone-pair electrons associated with the heterocyclic nitrogen atom fill the empty dangling bond of a silicon adatom via a dative bond.

Finally, in presence of one boron-defect, the possibility of a “forced” dative bond, corresponding to a chemical bond formation between the PAB molecule and the silicon electron occupied dangling bond, is emphasized.

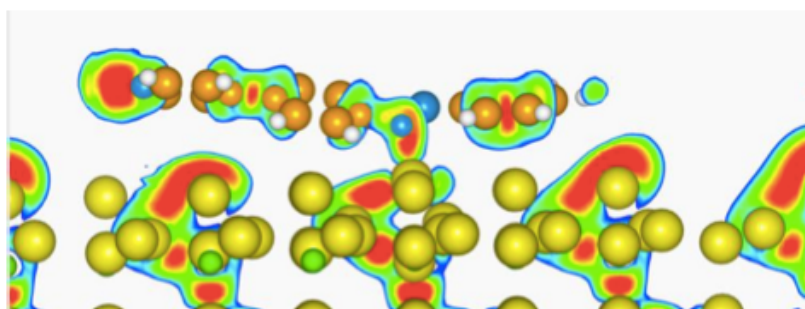


Fig. 1: Side view of the electron localisation function (ELF) for a parallel PAB adsorption model on a boron silicon surface.

### REFERENCE

1. K. Boukari, E. Duverger and Ph. Sonnet, Phys. Chem. Chem. Phys. 16 (2014) 24866.