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Doping of the hydrogen-passivated Si(100) surface by carborane films studied using density functional theory

Doping is a key process in semiconductor industry, in which the host electronic structure and carrier concentration are modified. When the semiconductor is doped, doping elements with the required electronic properties are introduced into its structure. Dopant introduction processes are either based on diffusion from gaseous phase or on ion implementation, where doping agents are implemented inside the host Si matrix through a high-energy bombardment. However, such a procedure has destructive effects on the structure of the Si matrix, especially near the surface1. It is therefore appropriate to be interested in alternative non-destructive methods such as a monolayer doping2,3 employing chemical reactions to bind a monolayer of dopant-rich molecules onto the surface of the host semiconductor. Such a monolayer can be formed, for example, from dithiocarboranes, i.e. molecules with a large permanent dipole capable of easily forming stable monolayers on a variety of substrates4–7.

Here we use Density Functional Theory to investigate the doping of hydrogen-passivated Si(100) substrates through the adsorption of dithiocarborane molecules. We find that dithiocarboranes can both physisorb and chemisorb on the substrate. Chemisorbed structures arise when a S atom in the molecular linker group replaces a surface H atom. We establish the formation of these Si-molecule bonds and characterize their mechanical and thermal stability. Analysis of the calculated electronic structure of adsorbed interfaces shows that carborane adsorption does not result in interface gap states. The band gap in adsorbed junctions is defined by Si states and its magnitude is almost unchanged with respect to the clean Si slab. The large carborane electrostatic dipole results in the downwards shift of Si spectral features by 0.3 eV, reducing the hole injection barrier by this amount with respect to the pristine Si substrate. Molecular dynamics simulations reveal these structural and electronic features to be stable at room temperature. Our work shows that molecular adsorbates having large electrostatic dipoles are a promising strategy to non-destructively dope semiconductor substrates.

References

1. Chen, W., Qi, D., Gao, X. & Wee, A. T. S. Surface transfer doping of semiconductors. Progress in Surface Science 84, 279–321 (2009).

2. Ye, L. et al. Boosting the Boron Dopant Level in Monolayer Doping by Carboranes. ACS Appl. Mater. Interfaces 7, 27357–27361 (2015).

3. Veerbeek, J. & Huskens, J. Applications of Monolayer-Functionalized H-Terminated Silicon Surfaces: A Review. Small Methods 1, 1700072 (2017).

4. Thomas, J. C. et al. Acid–Base Control of Valency within Carboranedithiol Self-Assembled Monolayers: Molecules Do the Can-Can. ACS Nano 12, 2211–2221 (2018).

5. Vetushka, A. et al. Adsorption of oriented carborane dipoles on a silver surface: Adsorption of oriented carborane dipoles on a silver surface. physica status solidi (b) 253, 591–600 (2016).

6. Baše, T. et al. Carboranedithiols: Building Blocks for Self-Assembled Monolayers on Copper Surfaces. Langmuir 28, 12518–12526 (2012).

7. Serino, A. C. et al. Work Function Control of Germanium through Carborane-Carboxylic Acid Surface Passivation. ACS Appl. Mater. Interfaces 9, 34592–34596 (2017).

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