Structural, electronic and optical properties of ordered 9,10-PQ monolayers on Si(001) surface

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Within the last years extensive efforts have been devoted to functionalizing semiconductor surfaces by organic molecules. Ordered monolayers may serve as a starting point to alter surface optical and electronic properties in specific ways in order to eventually realize applications such as molecular electronic devices or organic sensors. Besides, there have been comprehensive experimental and theoretical studies on the optical properties of relevant clean semiconductur surfaces. Especially measuring the reflectance anisotropy spectra (RAS) turned out to provide useful informations on the individual surface reconstructions. In recent works [1, 2] the influence of adsorption of a π-conjugated molecule (9,10-phenanthrenequinone) on electronic properties and RAS signal of the Si(001) surface was investigated.
We performed *ab-initio* calculations of this adsorbate-surface-system within the framework of gradient-corrected density functional theory (DFT-GGA), using a plane wave basis set and ultrasoft pseudopotentials to determine the structurally relaxed ground state. Optical properties are then calculated within the independent-particle approximation from all-electron wave functions obtained by the projector augmented wave method (PAW). We present the energetically most favored structural configurations and the respective RAS spectra for several degrees of coverage, discuss the character of the molecule-substrate bonds from a molecular orbital point of view and the origin of the distinct RAS features due to molecular and surface contributions.

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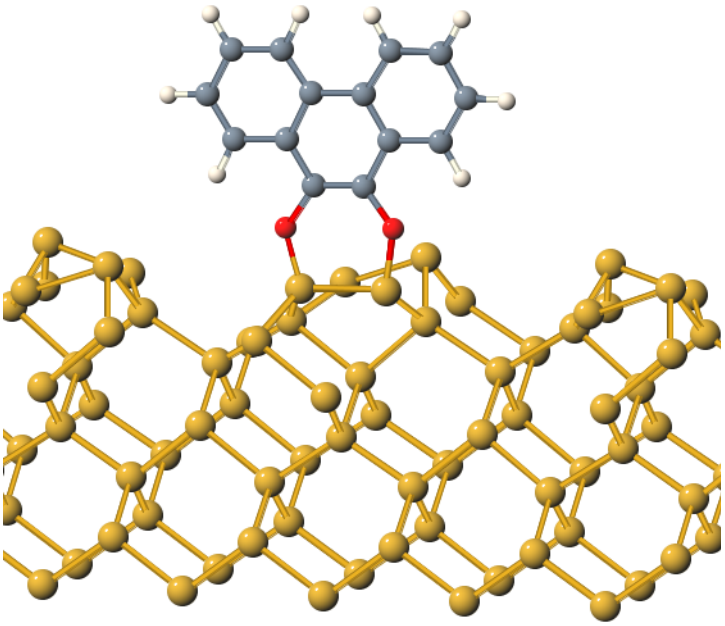

Figure 1: Energetically favored bonding configuration

References

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[2] C. A. Hacker and R. J. Hamers. Optical and Electronic Anisotropy of a π-Conjugated Molecular Monolayer on Silicon(001) Surface. *J. Phys. Chem. B*, 107:7689–7695, 2003.