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Metal deposition onto biomolecular layers on silicon surfaces: a study of interface formation using Raman spectroscopy

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Abstract

In this work the interface formed between the DNA base cytosine and hydrogen passivated Si(1 1 1) substrates is investigated by spectroscopic methods and density functional calculations of optimized adsorbate geometries. The cytosine was thermally evaporated by organic molecular beam deposition onto flat and vicinal H-passivated Si(1 1 1) substrates under ultra-high vacuum (UHV) conditions. In order to take advantage of surface-enhanced Raman scattering at rough metal surfaces, silver was evaporated onto the biomolecular adsorbate. Polarisation-dependent Raman measurements reveal that the cytosine molecules align along the steps on vicinal H–Si(1 1 1) surfaces. The orientation of the molecular plane of the cytosine molecule deduced from the SER spectra can be well reproduced with density functional calculations of the optimized geometries of an adsorbed cytosine molecule at a step edge of H-passivated Si(1 1 1) slab. As the binding energy of cytosine at the substrate step is as large as −0.41 eV, one can conclude that the coverage with silver does not affect the preferential adsorption geometry of the cytosine molecule.

Author Keywords: Cytosine; Silver; Silicon; SERS; DFT

78.30 Jw; 78.66 Qn

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