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Interface properties of metal/cytosine/Si(1 1 1):H heterostructures studied by means of SERS and DFT

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Abstract

In this work the interface formation between cytosine and hydrogen-passivated Si(1 1 1) substrates, the growth of cytosine layers as well as the interface between a metal (In or Ag) and the cytosine layers are studied. Cytosine was thermally evaporated by organic molecular beam deposition (OMBD) onto H-passivated Si(1 1 1) substrates under ultra-high vacuum conditions. Metal deposition on monolayers ($\sim$0.4 nm) of cytosine leads to an enhancement of the Raman signal via the surface-enhanced Raman scattering (SERS) effect. The interaction with metals is found to be very different due to the large difference in the ionisation potential of Ag and In (IP_{Ag} = 7.58 eV, IP_{In} = 5.78 eV). The signal enhancement arises mainly from contributions due to molecule–metal charge transfer. Density functional theory calculations were employed for modelling the interaction of metal atoms with cytosine. Computational approaches were carried out on silver–cytosine and indium–cytosine complexes using the B3LYP density functional with the LANL2DZ basis set.

Author Keywords: Cytosine; Si(1 1 1); In; Ag; SERS; DFT(B3LYP/LANL2DZ)

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