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Vacuum ultraviolet spectroscopic ellipsometry investigations of guanine layers on H-passivated Si(1 1 1) surfaces

S. D. Silaghi, a, M. Friedrich[a], R. Scholz[a], T. U. Kampen[a], C. Cobet[b], N. Esser[b], W. Richter[b], W. Braun[c] and D. R. T. Zahn[a]

[a] Institut für Physik, Technische Universität Chemnitz, D-09107, Chemnitz, Germany
[b] Institut für Festkörperphysik, Technische Universität Berlin, D-10623, Berlin, Germany
[c] BESSY GmbH, Albert-Einstein-Straße 15, D-12489, Berlin Adlerhof, Germany

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Abstract

Guanine layers deposited by organic molecular beam deposition onto H-passivated Si(1 1 1) substrates under ultra-high vacuum conditions were investigated by means of vacuum ultraviolet spectroscopic ellipsometry. The experimental absorption bands are compared to the transition energies calculated for a single guanine molecule using time-dependent density functional theory in the 6-31G(d) variational basis set at the B3LYP level of theory. Taking into account that the imaginary part of the effective dielectric function measured in ellipsometry is affected by thickness interferences and the impact of the substrate, the calculated oscillator strengths of the higher transition energies are in reasonable agreement with the experimental features.

Author Keywords: Guanine; Si(1 1 1); Vacuum ultraviolet spectroscopic ellipsometry; TD-DFT(B3LYP/6-31G(d))

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