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Optical dielectric function of $Si(bzimpy)_2$ – a hexacoordinate silicon pincer complex determined by spectroscopic ellipsometry

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Abstract Tang and VanSlyke demonstrated light emission from the first practical electroluminescent device based on a double-organic-layer structure of tris(8-hydroxyquinoline)aluminum, Alq_3, and a diamine film in the late 80's [1]. Since then, organic light emitting diodes (OLED) based on metal chelates such as Alq_3 have been widely studied. Despite the widespread use of Alq_3, there has been a broad search for new materials with improved properties, in particular, with respect to their chemical and electrochemical stability [2].

We have recently reported on the successful synthesis of a neutral, hexacoordinate silicon-based fluorescent complex $Si(bzimpy)_2$ [3]. Our results indicate that $Si(bzimpy)_2$ exhibits inherent advantages such as the tunability of the luminescence in the visible spectrum, greater thermal stability, and high charge mobility that is comparable to that of Alq_3. Despite the successful synthesis and encouraging electroluminescence at 560 nm the complex dielectric function of the water stable complex has not been reported yet.

Here we present spectroscopic ellipsometry data which were obtained from a $Si(bzimpy)_2$ thin-film in the spectral range from 300 nm to 1900 nm. A parameterized model dielectric function composed of a Tauc-Lorentz and Gaussian oscillators is employed to analyze the experimental ellipsometry data. We find a good agreement between the critical point energies observed experimentally and our density functional theory calculations reported recently [3].

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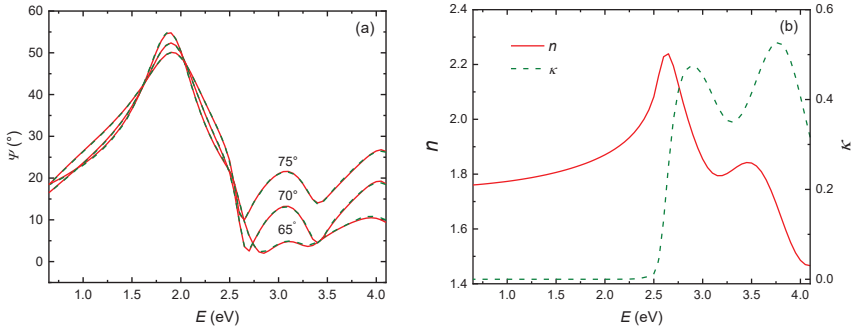

Fig. 1 (a) Experimental (green dashed line) and best-model (red solid line) Ψ-spectra for a Si(bzimpy)$_2$ thin-film sample measured at three different angles of incidence $\Phi_a = 65°, 70°$, and $75°$ in spectral range from 0.65 eV to 4.1 eV. An excellent agreement between the experimental and best-model calculated data is obtained using the optical constants shown in Fig. 1(b).
(b) The best-fit model refractive index n (red solid line) and extinction coefficient κ (green dashed line) of Si(bzimpy)$_2$ in the spectral range from 0.65 eV to 4.1 eV. The spectrum above the band gap at 2.51 eV is dominated by absorption bands which are in good agreement with DFT calculations [3].

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