UNDERSTANDING POLYMER ORIENTATION AT THE INTERFACE BY SERS

A. Harbuzaru[1], I. Arrechea-Marcos[1], J.T. López Navarrete[1], R. Ponce Ortiz[1], M.C. Ruiz Delgado[1]

[1] Department of Physical Chemistry, Malaga University, Malaga, 29071, Spain, harbalexandra07@gmail.com

Key Words: *SERS, Raman, P(NDI2OD-T2)*

In the organic electronic research field, it is well known that the largest contribution to charge transport occurs within the first few nanometers of the semiconductor near the dielectric interface. Surface Enhanced Raman spectroscopy (SERS) appears as an easy and straightforward technique to analyze this buried interface and to provide useful information on molecular orientation at the device active layer. [1, 2]

Here we present the study of the molecular orientation of the widely studied P(NDI2OD-T2) polymer [3] at the semiconductor/dielectric and semiconductor/metal interfaces using SERS and DFT calculations. Our first SERS results show a relative intensification of selected normal modes, which indicates that the orientation of the polymer changes from a *face-on* (before annealing treatment) to and *edge-on* disposition after melt annealing, being this in good agreement with the previous results gathered from other techniques (Figure 1). [4-7]

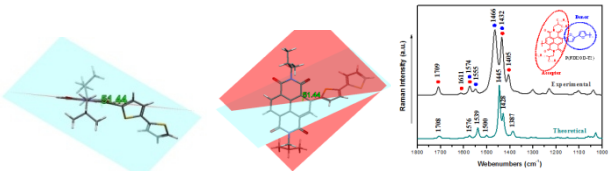

Figure 1: a) DFT predicted chemical structure of the P(NDI2OD-T2) comonomeric units, with indication of the key dihedral angle, b) Comparison between experimental and theoretical B3LYP/6-31G** Raman spectra of P(NDI2OD-T2).

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