Deciphering molecular mechanisms of interface buildup and stability in porous Si/eumelanin hybrids

Elisa Pinna 1,2*, Claudio Melis 1,2*, Aleandro Antidormi 1,2, Roberto Cardia 1, Elisa Sechi 1, Giancarlo Cappellini 1, Marco d’Ischia 3, Luciano Colombo 1,2 and Guido Mula 1,2

1 Dipartimento di Fisica, Università degli Studi di Cagliari, S.P. 8 km 0.700, 09042 Monserrato (Ca), Italy – e-mail: guido.mula@unica.it
2 Istituto Officina dei Materiali CNR-IOM, unità di Cagliari SLACS, Cittadella Universitaria di Monserrato, S.P. 8 km 0.700, 09042 Monserrato (Ca) – e-mail: luciano.colombo@dsf.unica.it
3 Department of Organic Chemistry and Biochemistry, University of Naples “Federico II”, Via Cintia 4, 80126 Naples, Italy - e-mail: dischia@unina.it
* Correspondence: elisa.pinna@dsf.unica.it - +39 070 6754787; claudio.melis@dsf.unica.it - +39 070 6754929

Figure S1: Absorbance spectra as a function of time for two different concentrations of DHI in EtOH. (a) 0.25 mg/mL and (b) 0.12 mg/mL. The vertical axis has been kept identical to that of Figure 5 for easier comparison.
Figure S2. Analysis of the evolution of the absorbance spectra of the DHI in EtOH solutions shown in Figure S1 at three different spectral positions: 330 nm, 460 nm and 780 nm. The curves represent the normalized evolution of the absorbance for (a) 0.25 mg/mL and (b) 0.12 mg/mL.

Figure S3. Comparison between the calculated spectra for the PT structure (blue line) and the experimental absorption of 0.25mg/mL solution of DHI in EtOH (red line, curve corresponding to the absorbance of after 600').
Figure S4. Comparison of the theoretical/computational spectrum for the PT structure calculated in this work with that reported by Meng and Kaxiras [44].