

Supplementary Information: A Spectroscopic Characterization of Charge Carriers of the Organic Semiconductor Quinacridone Compared with Pentacene during Redox Reactions

Sandra Enengl,^{*ab} Christina Enengl,^{ab} Sandra Pluczyk,^c Eric D. Glowacki,^b Mieczyslaw Lapkowski,^{cd} Eitan Ehrenfreund,^e Helmut Neugebauer,^b and Niyazi Serdar Sariciftci^b

1 Reversibility of pentacene and quinacridone upon oxidation reaction

The re-reduction of pentacene and quinacridone is shown in Figure S1 and Figure S2, respectively. In case of pentacene potentials between 1300 mV and 0 mV have been applied. The spectrum obtained at 0 mV (the potential before oxidation starts) is taken as a reference spectrum for the difference spectra shown in Figure S1. As can be seen from this Figure almost no changes occur anymore, showing an irreversible process.

In Figure S2 difference spectra for the re-reduction reaction of quinacridone are shown by applying potentials between 1700 mV and 0 mV. Again the potential at 0 mV (the potential before oxidation starts) is taken as reference spectrum. The re-reduction reaction shows a quite reversible process. Although one would expect an increase in absorption at the beginning of the re-reduction reaction (which can be correlated to the reversibility of the second oxidation peak), a steady decrease in absorption of the broad band is observed. The continuous decrease of absorption spectra is explained due to superposition of the first and the second re-reduction peak, because it appears as one main peak in the cyclic voltammogram, see Figure 1 (c). However, at the beginning of the re-reduction reaction the decrease in absorption values is less pronounced than in the course of the re-reduction.

2 Reversibility of pentacene and quinacridone upon reduction reaction

The re-oxidation reaction for both investigated compounds has been carried out in the same way as re-reduction reaction. Figure S3 shows the difference spectra for pentacene by changing the potential between -1700 mV and 0 mV, taking 0 mV (the potential before reduction starts) as reference spectrum. These spectra indicate an irreversible process for the re-oxidation reaction, because the spectral behavior from the pristine material is not obtained anymore.

The situation for quinacridone is different. Figure S4 depicts difference spectra during re-oxidation of quinacridone. The potential has been changed in the range between -2100 mV and 0 mV, taking 0 mV (the potential before reduction starts) as reference spectrum. As re-oxidation starts, the absorption value of the broad band decreases demonstrating reversibility.

^a Institute of Polymer Science, Johannes Kepler University Linz, Altenbergerstraße 69, 4040 Linz, Austria. E-mail: Sandra.Enengl@jku.at

^b Linz Institute for Organic Solar Cells (LIOS), Physical Chemistry, Johannes Kepler University Linz, Altenbergerstraße 69, 4040 Linz, Austria.

^c Department of Physical Chemistry and Technology of Polymers, Faculty of Chemistry, Silesian University of Technology, 9 Marcina Strzody street, 44-100 Gliwice, Poland.

^d Center of Polymer and Carbon Materials, Polish Academy of Sciences, 34 M. Curie-Skłodowskiej street, 41-819 Zabrze, Poland.

^e Department of Physics and Solid State Institute, Technion-Israel Institute of Technology, Technion City, 32000 Haifa, Israel.

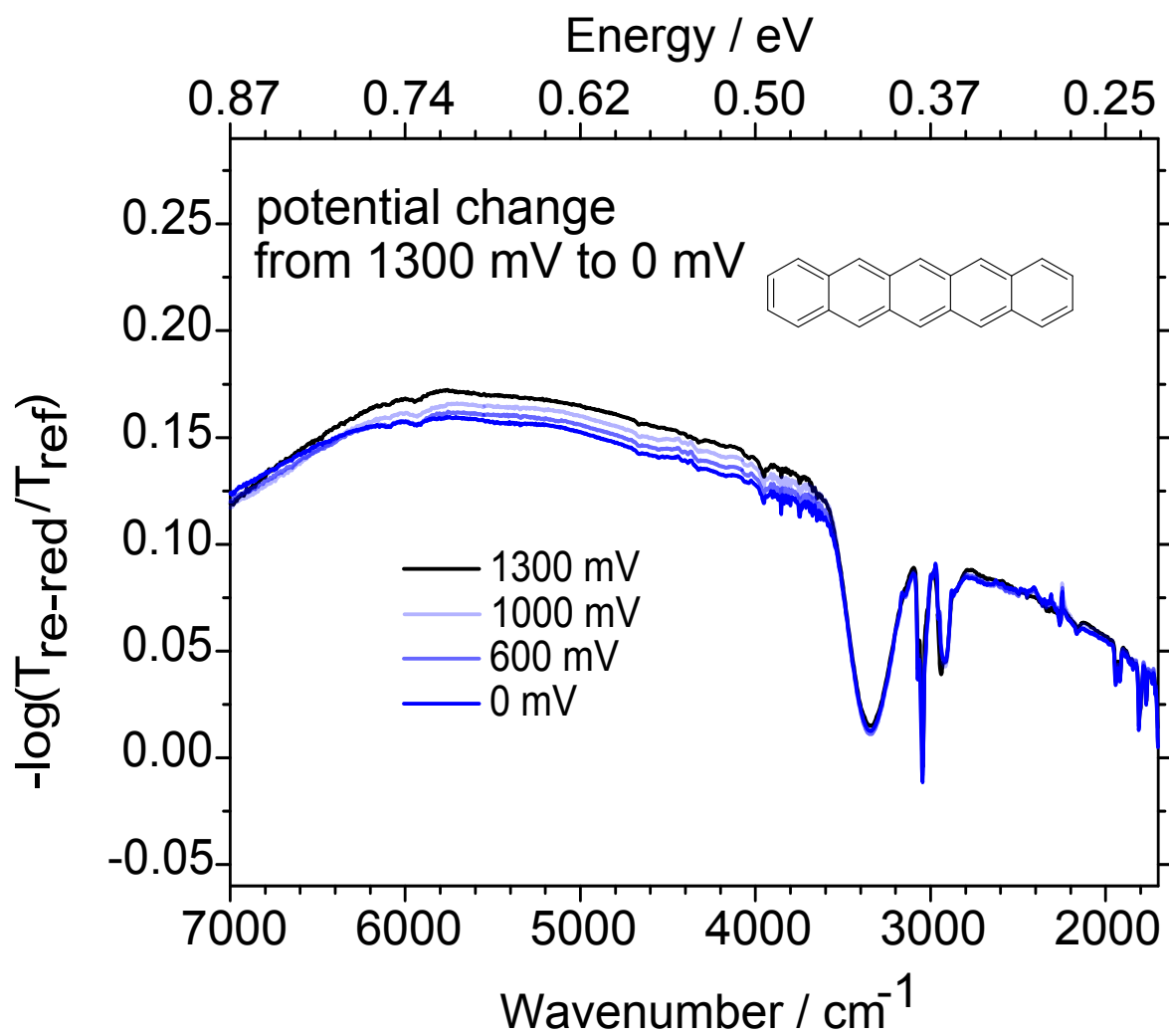


Fig. S1 Difference spectra are shown by changing potentials between 1300 mV and 0 mV taking 0 mV (the potential before oxidation starts) as reference spectrum. The oxidation reaction of pentacene indicates an irreversible process, because spectra do not show the spectral behavior of the pristine material.

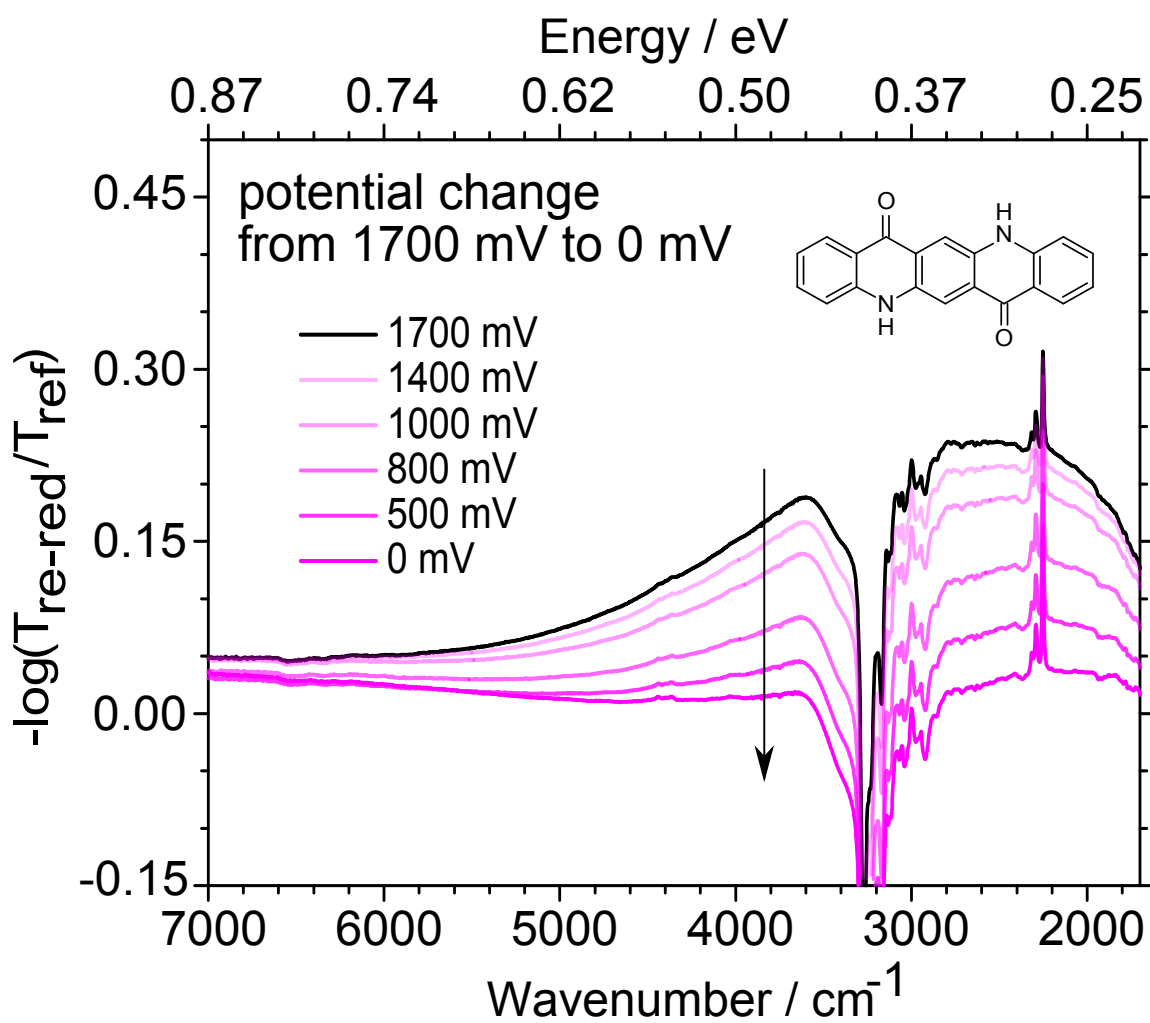


Fig. S2 Difference spectra by changing potentials between 1700 mV and 0 mV taking 0 mV (the potential before oxidation starts) as reference spectrum. The oxidation reaction demonstrates reversibility of quinacridone.

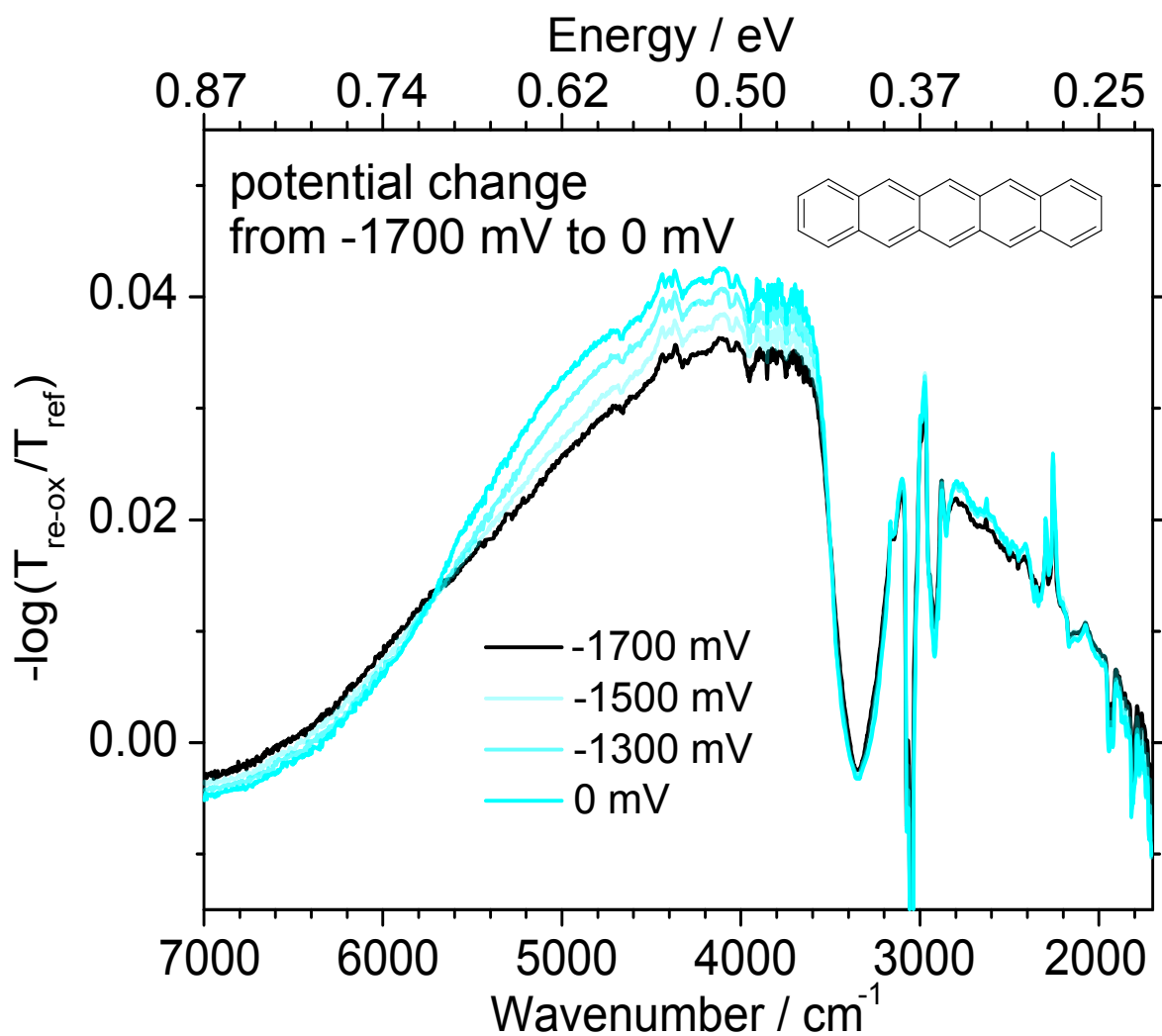


Fig. S3 Difference spectra by changing potentials between -1700 mV and 0 mV taking 0 mV (the potential before reduction starts) as reference spectrum. The reduction reaction of pentacene indicates an irreversible process, because spectra do not show the spectral behavior of the pristine material.

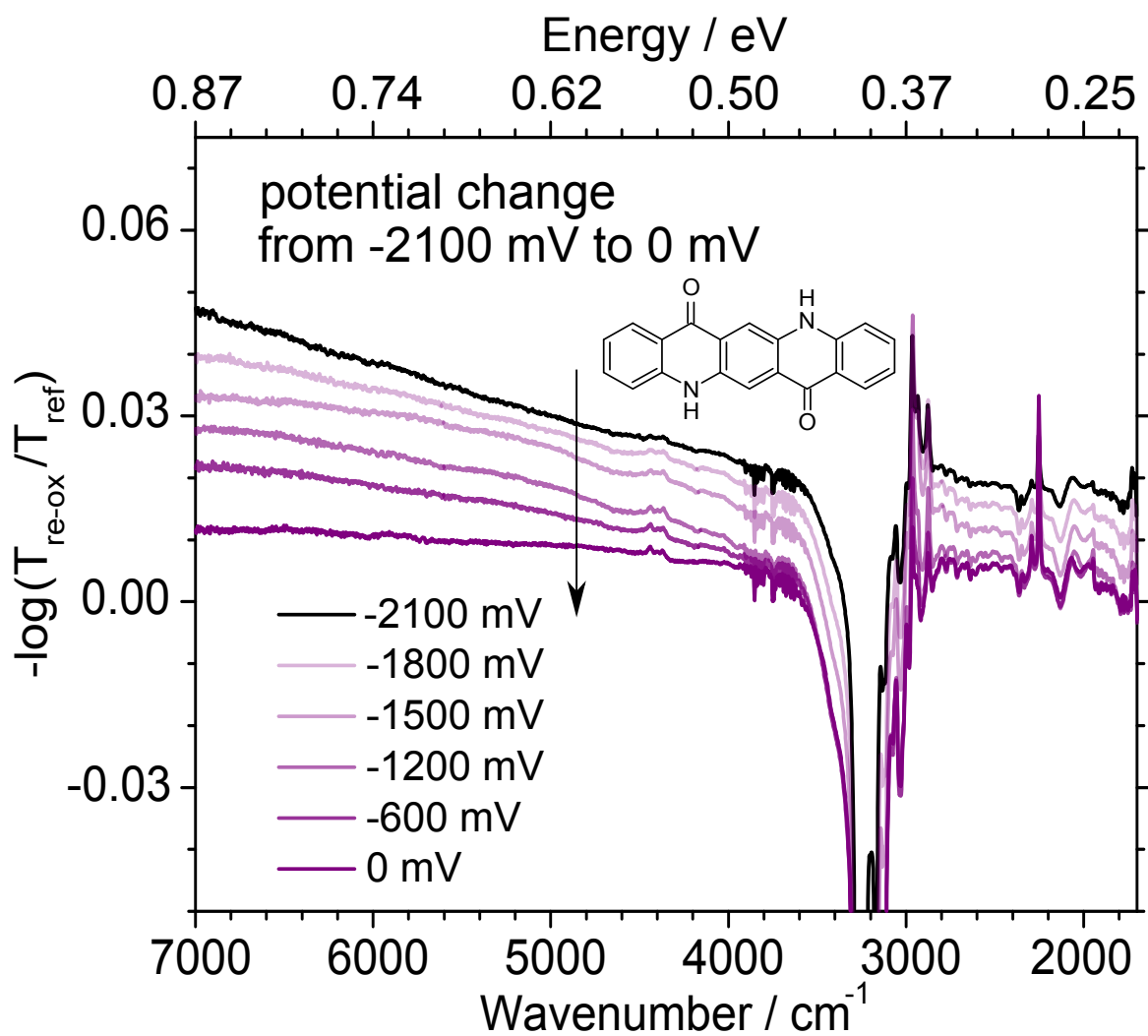


Fig. S4 Difference spectra by changing potentials between -2100 mV and 0 mV taking 0 mV (the potential before reduction starts) as reference spectrum. The reduction reaction demonstrates reversibility of quinacridone.