

## Supporting Information

for

### **X-Ray spectroscopy characterization of self-assembled monolayers of nitrile-substituted oligo(phenylene ethynylene)s with variable chain length**

Hicham Hamoudi,<sup>1</sup> Ping Kao,<sup>2</sup> Alexei Nefedov,<sup>3</sup> David L. Allara,<sup>2</sup> and Michael Zharnikov\*<sup>1,§</sup>

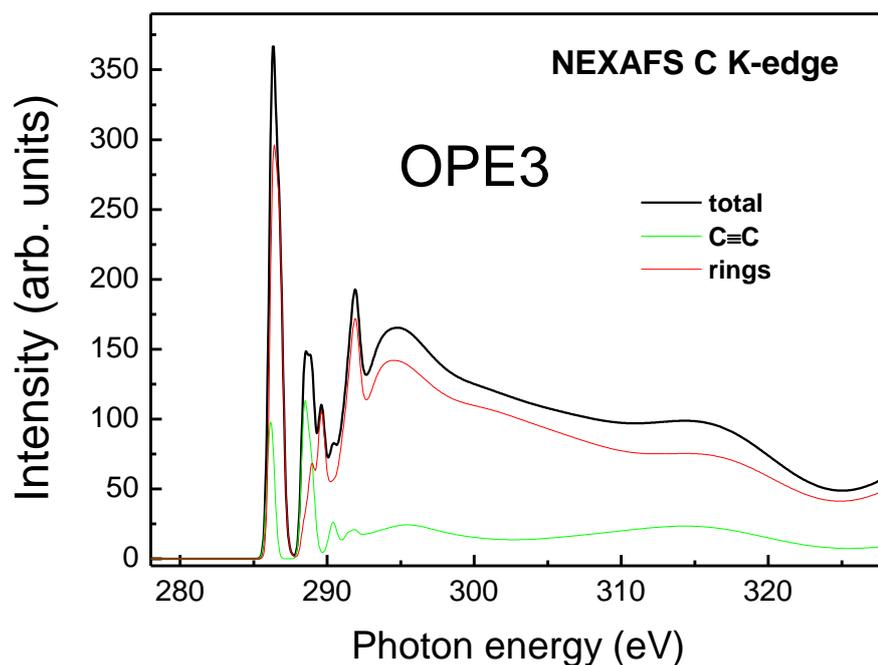
Address: <sup>1</sup>Angewandte Physikalische Chemie, Universität Heidelberg, D-69120 Heidelberg, Germany; <sup>2</sup>Departments of Chemistry and Material Science, Pennsylvania State University, University Park, PA16802, USA and <sup>3</sup>Institut für Funktionelle Grenzflächen, Karlsruher Institut für Technologie, Eggenstein-Leopoldshafen, D-76344, Germany

Email: Michael Zharnikov\* - Michael.Zharnikov@urz.uni-heidelberg.de

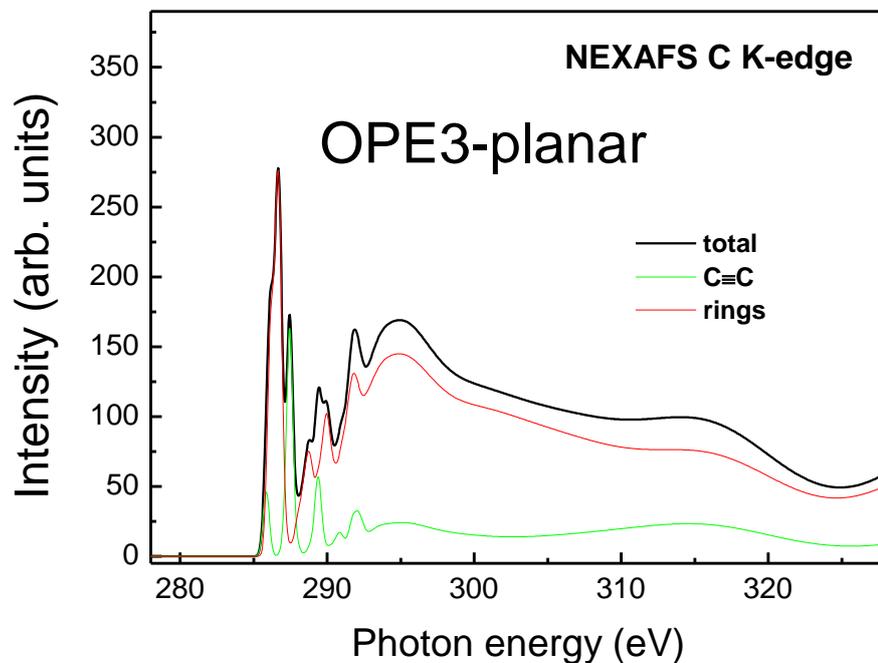
\*Corresponding author

§Phone: +49-6221-54 4921, Fax: +49-6221-54 6199

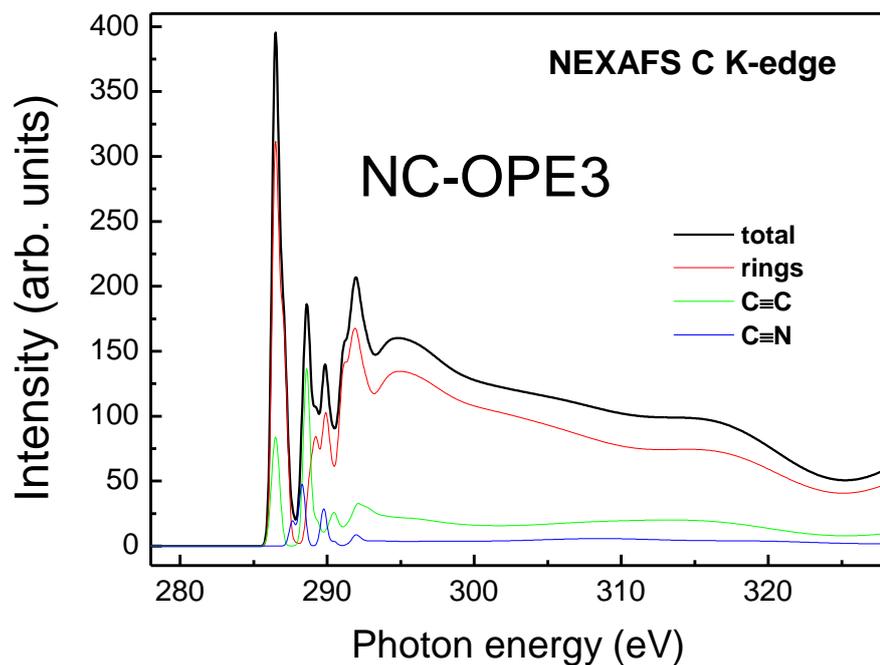
### **Calculated X-ray absorption spectra**



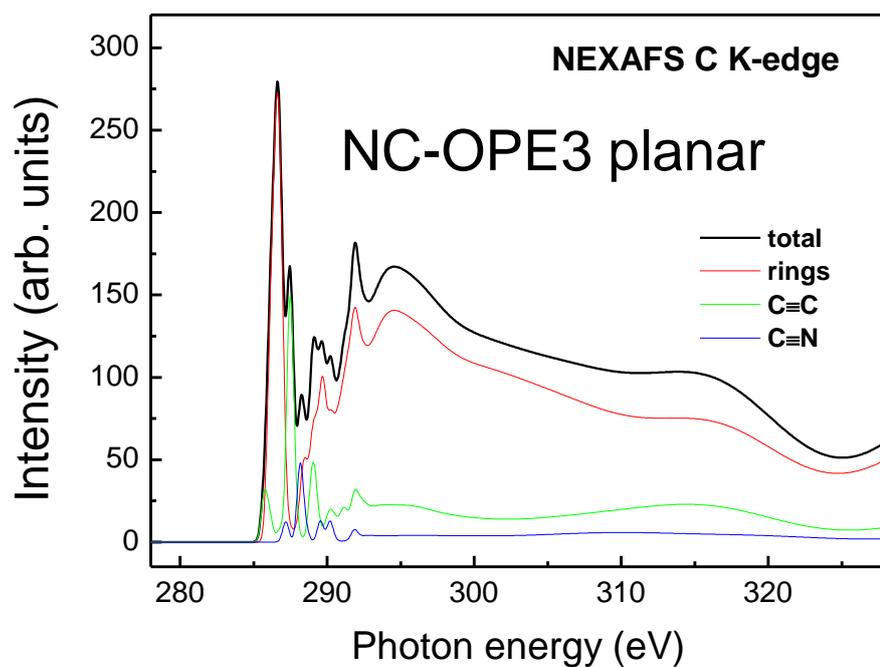
**Figure S1:** Calculated C K-edge NEXAFS spectra of OPE3 in the twisted conformations. The spectrum is decomposed into the contributions related to the individual functional units.



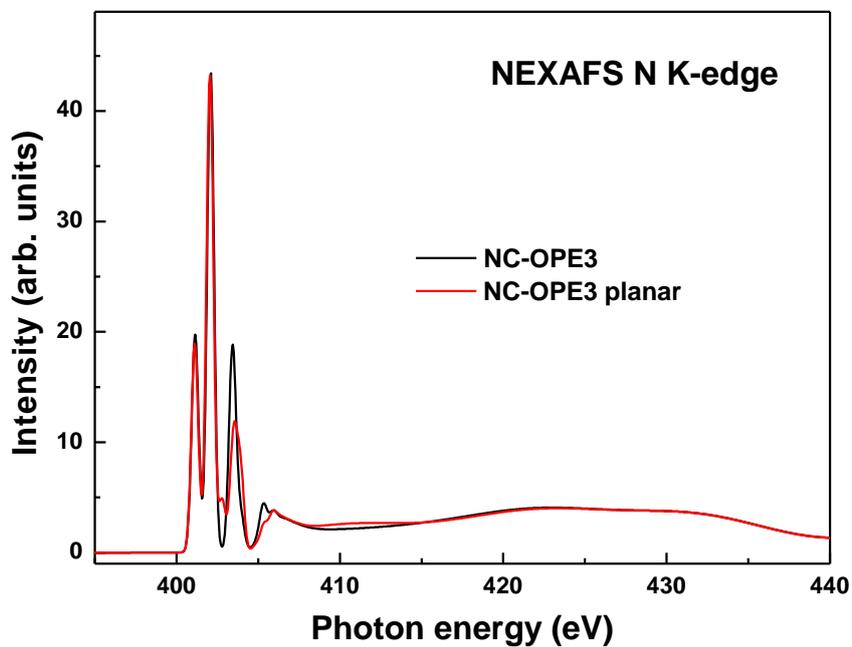
**Figure S2:** Calculated C K-edge NEXAFS spectra of OPE3 in the planar conformations. The spectrum is decomposed into the contributions related to the individual functional units.



**Figure S3:** Calculated C K-edge NEXAFS spectra of NC-OPE3 in the twisted conformations. The spectrum is decomposed into the contributions related to the individual functional units.



**Figure S4:** Calculated C K-edge NEXAFS spectra of NC-OPE3 in the planar conformations. The spectrum is decomposed into the contributions related to the individual functional units.



**Figure S5:** Calculated N K-edge NEXAFS spectra of NC-OPE3 in the planar and twisted conformations.