Electronic Structure of Low-Dimensional Carbon Π-Systems - DTU Orbit (09/11/2017)

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X-ray absorption spectroscopy (XAS) is combined with density functional theory (DFT) to determine the orbitals of one- and two-dimensional carbon Π-systems (lycopene, beta-carotene, retinal, retinol, retinoic acid, coronene, triphenylene). Considerable fine structure is observed for the transition from the C is level to the lowest unoccupied molecular orbital (LUMO) and explained by DFT. The wave functions of the one-dimensional chain molecules display the node structure of a vibrating string. The XAS transition energy is decomposed into contributions from the C is core level, the Π* final state, and the electron hole interaction. For the latter, we develop a simple model that accurately represents a full Delta-self-consistent field (ΔSCF) calculation. The distortion of the LUMO because of its interaction with the C is hole is investigated. These results illustrate the electronic states of prototypical Π-bonded carbon structures with low-dimensional character, such as those used in molecular complexes for solar cells, confined graphene structures, and molecular wires.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Wisconsin-Madison, Lawrence Berkeley National Laboratory, Max Planck Institute for the Structure and Dynamics of Matter
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Number of pages: 7
Pages: 12362-12368
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Physical Chemistry C
Volume: 120
Issue number: 23
ISSN (Print): 1932-7447
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.438 SNIP 1.356
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.128 SNIP 1.417
Web of Science (2009): Indexed yes

BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.856 SNIP 1.033
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2004): Indexed yes
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Web of Science (2001): Indexed yes
Web of Science (2000): Indexed yes
Original language: English
DOIs:
10.1021/acs.jpcc.6b02530
Source: FindIt
Source-ID: 2304495333
Publication: Research - peer-review › Journal article – Annual report year: 2016