

Front end for the model and its Output

The screenshot shows a dark-themed web application window titled "AI Paper Review & Summary". At the top, there's a header bar with a logo, a search icon, and a "Deploy" button. Below the header, a navigation bar includes links to "Dell", "Ramayan - Full Ani...", "Gmail", "YouTube", "Maps", "Venom - iBOMMA", and "McAfee Security". A sidebar on the left has icons for "Upload Research PDFs", "Drag and drop files here Limit 200MB per file +PDF", and a file named "pubs1.pdf 3.1MB". The main content area features a section titled "Normalized Text Preview" with the heading "Normalized Text Preview". It contains a "Processed Content" box with abstract text about micro-cocrystals of intermolecular charge-transfer (CT) complexes formed from pyrene and tetracyanobenzene. Below the abstract is a "Generate Summary & Review" button. At the bottom of this section is a "Paper Summary" button. The bottom of the screen shows a Windows taskbar with various pinned icons and system status indicators.

This screenshot shows the same application window after interacting with the "Paper Summary" button. The main content area now displays a detailed "Paper Summary" section. It begins with a paragraph about the heavy-metal complexes used in TTA-UC systems. It then lists the corresponding authors (Jianlei Han, Pengfei Duan, Zhaohu Xu), their institutions (Jiaxing University, National Center for Nanoscience and Technology, Beijing 100190, China Academy of Sciences), and their ORCID IDs. The summary continues with information about the research work, mentioning grants from the National Natural Science Foundation of China and the Chinese Academy of Sciences. It also discusses the chemical structures of the CT sensitizer complex, spin density distribution, and photophysical properties of the system. The bottom of the screen shows a Windows taskbar with pinned icons and system status indicators.

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AI Paper Review & Summary

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Abstract

ABSTRACT: Micro-cocrystals of the intermolecular charge-transfer (CT) complex formed from pyrene and tetracyanobenzene can be fabricated via a solution-based method.

Critique: Section is brief, | Needs more structured sentences.

Methods

Experimental details, kinetics analysis details, and photophysical properties of pyrene and TCNB (PDF) ■ AUTHOR INFORMATION Corresponding Authors Jianlei Han - College of Biological and Chemical Engineering, Jiaxing University, Jiaxing 314001, China; orcid.org/0000-0001-6566-7621; Email: hanjianlei@jxu.edu.cn Pengfei Duan - Laboratory of Nanosystem and Hierarchical Fabrication, National Center for Nanoscience and Technology, Beijing 100190, China; University of Chinese Academy of Sciences, Beijing 101408, China; orcid.org/0000-0002-5971-7546; Email: duangf@nаноctr.cn Zihao Xu - Beijing National Laboratory for Molecular Sciences, Huairou Research Center, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China; orcid.org/0000-0003-0805-8533; Email: zihaoxu@iccas.ac.cn Authors Zhiyang Bai - Beijing National Laboratory for Molecular Sciences, Huairou Research Center, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China Jiao Mu - Beijing National Laboratory for Molecular Sciences, Huairou Research Center, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China Xuefeng Yang - Laboratory of Nanosystem and Hierarchical Fabrication, National Center for Nanoscience and Technology, Beijing 100190, China; orcid.org/00090001-9921-0176 Tonghan Zhao - Laboratory of Nanosystem and Hierarchical Fabrication, National Center for Nanoscience and Technology, Beijing 100190, China Yonghong Shi - Xi'an Rare Metal Materials Institute Co., Ltd., Northwest Institute for Non-ferrous Metal Research, Xi'an 710016, China Complete contact information is available at: <https://pubs.acs.org/doi/10.1021/jacs.5c17410> Notes: The authors declare no competing financial interest. ■ ACKNOWLEDGMENTS This work was supported by National Natural Science Foundation of China (22588301, 22405215, 22302046, 22205045, 22172041, 52173159, 92356307, and 22403097), the National Key Basic R&D Research Program of Ministry of Science and Technology of the People's Republic of China (2021YFA1200303), and the Strategic Priority Research Program of the Chinese Academy of Sciences (XDB0960000, XDB0960200, XDB0960201). This work exemplifies a novel approach to CT exciton triplet sensitization and offers valuable insights into the precise engineering of triplet exciton properties via CT interaction design. ■ ASSOCIATED CONTENT ■ Supporting Information The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/jacs.5c17410>. Although upconversion quantum yield could not be determined due to challenges in quantifying absorbed photons, these results, to the best of our knowledge, provide the first experimental demonstration of CT exciton utilization in TTAUC systems and establish a viable pathway for heavy atom-free triplet sensitizer development.

Results

Although upconversion quantum yield could not be determined due to challenges in quantifying absorbed photons, these results, to the best of our knowledge, provide the first experimental demonstration of CT exciton utilization in TTAUC systems and establish a viable pathway for heavy atom-free triplet sensitizer development. This electronic transition was further confirmed by TD-DFT calculations (Figure S4 and Table S1); the HOMO + LUMO excitation, corresponding to the lowest-energy CT transition with an oscillator strength of 0.0036 (2.7 eV, 461 nm) agrees well with the experimental result (2.5 eV, 500 nm). In summary, we have observed the intersystem crossing of CT excitons generated in the Py-TCNB cocrystal, enabling efficient triplet energy transfer from the resulting triplet CT excitons to a DPA-based liquid annihilator, which yields upconverted emission through the TTA. Subsequently, TTA between two triplets of 2 produces a singlet excited state, resulting in a blue fluorescence emission (Figure 1 f). Increased upconversion performance for thin film solar cells: a trimolecular composition.

Critique: Quality acceptable.

Limitations

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INFORMATION Corresponding Authors: Jianlei Han - College of Biological and Chemical Engineering, Jiaxing University, Jiaxing 314001, China; orcid.org/0000-0001-6566-7621; Email: hanjianlei@jxu.edu.cn Pengfei Duan - Laboratory of Nanosystem and Hierarchical Fabrication, National Center for Nanoscience and Technology, Beijing 100190, China; University of Chinese Academy of Sciences, Beijing 101408, China; orcid.org/0000-0002-5971-7546; Email: duangf@nаноctr.cn Zihao Xu - Beijing National Laboratory for Molecular Sciences, Huairou Research Center, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China; orcid.org/0000-0003-0805-8533; Email: zihaoxu@iccas.ac.cn Authors: Zhiyang Bai - Beijing National Laboratory for Molecular Sciences, Huairou Research Center, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China Jiao Mu - Beijing National Laboratory for Molecular Sciences, Huairou Research Center, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, China Xuefeng Yang - Laboratory of Nanosystem and Hierarchical Fabrication, National Center for Nanoscience and Technology, Beijing 100190, China; orcid.org/00090001-9921-0176 Tonghan Zhao - Laboratory of Nanosystem and Hierarchical Fabrication, National Center for Nanoscience and Technology, Beijing 100190, China Yonghong Shi - Xi'an Rare Metal Materials Institute Co., Ltd., Northwest Institute for Non-ferrous Metal Research, Xi'an 710016, China Complete contact information is available at: <https://pubs.acs.org/doi/10.1021/jacs.5c17410> Notes: The authors declare no competing financial interest. ■ ACKNOWLEDGMENTS This work was supported by National Natural Science Foundation of China (22588301, 22405215, 22302046, 22205045, 22172041, 52173159, 92356307, and 22403097), the National Key Basic R&D Research Program of Ministry of Science and Technology of the People's Republic of China (2021YFA1200303), and the Strategic Priority Research Program of the Chinese Academy of Sciences (XDB0960000, XDB0960200, XDB0960201). This work exemplifies a novel approach to CT exciton triplet sensitization and offers valuable insights into the precise engineering of triplet exciton properties via CT interaction design. ■ ASSOCIATED CONTENT ■ Supporting Information The Supporting Information is available free of charge at <https://pubs.acs.org/doi/10.1021/jacs.5c17410>. Although upconversion quantum yield could not be determined due to challenges in quantifying absorbed photons, these results, to the best of our knowledge, provide the first experimental demonstration of CT exciton utilization in TTAUC systems and establish a viable pathway for heavy atom-free triplet sensitizer development.

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