


 ACS Mobile is a mobile app for Android and Apple devices. [Find out more](#)

## Article

## Design of Efficient Ambipolar Host Materials for Organic Blue Electrophosphorescence: Theoretical Characterization of Hosts Based on Carbazole Derivatives

Dongwook Kim\*†, Veaceslav Coropceanu†, and Jean-Luc Brédas\*†

 School of Chemistry and Biochemistry, and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400, United States  
 Department of Chemistry, Kyonggi University, San 94-6 Iui-Dong, Yeongtong-Gu, Suwon 443-760, Korea

*J. Am. Chem. Soc.*, 2011, 133 (44), pp 17895-17900

DOI: 10.1021/ja207554h

Publication Date (Web): September 25, 2011

Copyright © 2011 American Chemical Society

[dongwook-kim@kgu.ac.kr](mailto:dongwook-kim@kgu.ac.kr); [jean-luc.bredas@chemistry.gatech.edu](mailto:jean-luc.bredas@chemistry.gatech.edu)

## Abstract

-  Full Text HTML
-  Hi-Res PDF [2174 KB]
-  PDF w/ Links [840 KB]

Your current credentials do not allow retrieval of the full text.

Purchase the full-text

PDF/HTML, figures/images, references and tables, (where available)

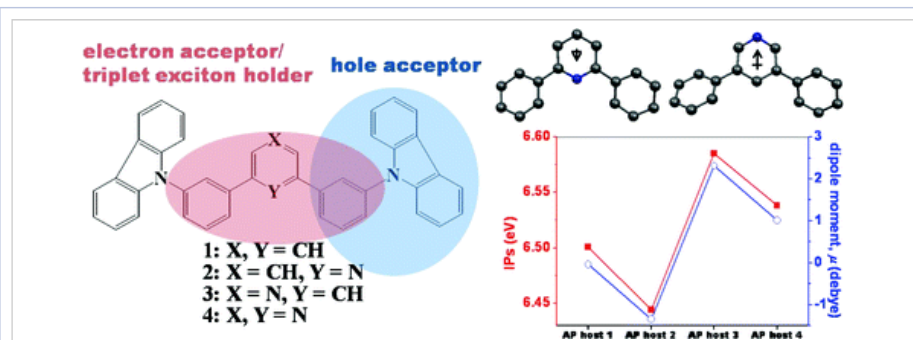


## #Author Status

Also affiliated with Department of Chemistry, King Abdulaziz University, Jeddah 21589, Saudi Arabia


 Section: Physical Organic Chemistry

## Abstract



Density functional theory calculations were carried out to investigate the electronic structures of representative ambipolar hosts for blue electroluminescence, based on two carbazole end groups and *meta*-terphenyl (*mTP*)-like bridges. The bridge molecular segments include *mTP*, 2,6-bisphenylpyridine, 3,5-bisphenylpyridine, and 2,6-bisphenylpyrimidine. While the ionization potentials and electron affinities of these molecules are mainly determined by their hole- and electron-transport subunits, respectively, each subunit impacts the electronic properties of the other upon their binding, mainly in an inductive way. Importantly, the lowest triplet state of the hosts is determined to be confined into the *mTP*-like bridges since these are the subunits with lowest individual triplet energy. Extension of the phenyl-based  $\pi$ -conjugated system via *meta* linkages is found to be effective in modulating the electron affinity value while maintaining a high triplet energy.

 View: [Full Text HTML](#) | [Hi-Res PDF](#) | [PDF w/ Links](#)

## Related Content

 Molecular Design and Ordering Effects in  $\pi$ -Functional Materials for Transistor and Solar Cell Applications  
*Journal of the American Chemical Society*








 Fine Tuning the Energetics of Excited-State Intramolecular Proton Transfer (ESIPT): White Light Generation in A Single ESIPT System  
*Journal of the American Chemical Society*

 Theoretical Investigation of Triscarbazole Derivatives As Host Materials for Blue Electrophosphorescence: Effects of Topology  
*Chemistry of Materials*

## Other ACS content by these authors:

[Dongwook Kim](#)  
[Veaceslav Coropceanu](#)  
[Jean-Luc Brédas](#)

## Tools

-  Add to Favorites
-  Download Citation
-  Email a Colleague
-  Permalink
-  Order Reprints
-  Rights & Permissions
-  Citation Alerts

## SciFinder Links



Get Reference Detail

Get Substances

Get Cited

Explore by:

- Author of this Article
- Any Author
- Research Topic  
(Now with patent search)



## History







 Published In Issue  
 November 09, 2011

 Article ASAP  
 October 13, 2011

 Just Accepted Manuscript  
 September 25, 2011

Received: August 10, 2011

## Recommend &amp; Share

-  ACS Network
-  Facebook
-  Tweet This
-  CiteULike
-  Newsvine
-  Digg This
-  Delicious

## Citing Articles

[View all 1 citing articles](#)

Citation data is made available by participants in [CrossRef's](#) Cited-by Linking service. For a more comprehensive list of citations to this article, users are encouraged to perform a search in [SciFinder](#).



1155 Sixteenth Street N.W.  
Washington, DC 20036

### Products

- [Journals A-Z](#)
- [Books](#)
- [C&EN](#)
- [C&EN Archives](#)
- [ACS Legacy Archives](#)
- [ACS Mobile](#)
- [Video](#)

### User Resources

- [About Us](#)
- [ACS Members](#)
- [Librarians](#)
- [Authors & Reviewers](#)
- [Website Demos](#)

### Support

- [Get Help](#)
- [For Advertisers](#)
- [Institutional Sales](#)

### Partners



### Search ACS Publications

Search Anywhere

**Search**