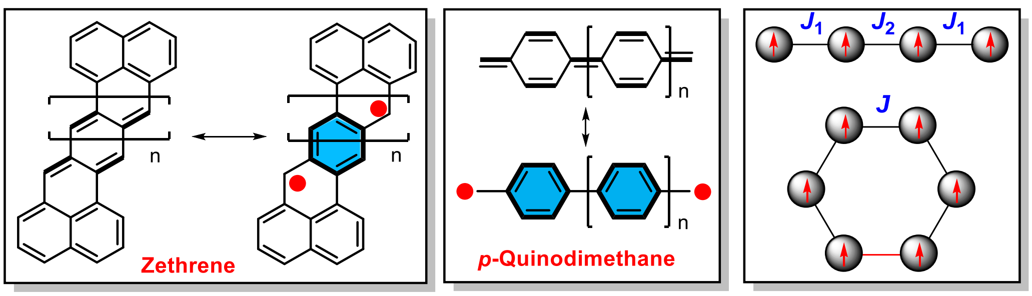
# From Open-shell Singlet Diradicaloids to Polyradicaloids

**Jishan Wu**

*Department of Chemistry, National University of Singapore, 3 Science Drive 3, 117543, Singapore; email: chmwuj@nus.edu.sg*

So far, most reported π-conjugated systems in neutral state have a closed-shell ground state. However, recent research disclosed that certain type of π-system could have open-shell singlet diradical and even polyradical ground state.[1] In this lecture, I will discuss various types of open-shell polycyclic hydrocarbons developed in our group: (a) zethrenes,[2] (b) extended *p*-quinodimethanes, [3] (c) linear and macrocyclic polyradicaloids,[4] (d) zigzag edged nanographenes/graphene nanoribbons,[5] and (e) 3D π-conjugated diradical cages and 2D covalent organic radical frameworks.[6] The discussion will mainly include their challenging synthesis, their characterizations of the ground-state structures, and their unique optical, electronic and magnetic properties. These fundamental studies now allow us to do rational design of stable open-shell singlet molecules with tunable physical properties and exploit their applications in molecular electronics, spintronics and photonics.[7]




## References:

[1] See our reviews and accounts: (a) Z. Sun *et al.*, *Chem. Soc. Rev.* **2012**, *41*, 7857. (b) Z. Sun *et al.*, *Acc. Chem. Res.* **2014**, *47*, 2582. (c) Z. Zeng *et al.*, *Chem. Soc. Rev.* **2015**, *44*, 6578. (d) T. Y. Gopalakrishna *et al.*, *Chem. Commun.* **2018**, *54*, 2389.

[2] (a) Z. Sun *et al.*, *J. Am. Chem. Soc.* **2011**, *133*, 11896. (b) Y. Li *et al.*, *J. Am. Chem. Soc.* **2012**, *134*, 14913. (c) Z. Sun *et al.*, *J. Am. Chem. Soc.* **2013**, *135*, 18299. (d) Y. Ni *et al.*, *Angew. Chem. Int. Ed.* **2016**, *55*, 2815. (e) W. Zeng *et al.*, *Angew. Chem. Int. Ed.* **2016**, *55*, 8816. (f) R. Huang *et al.*, *J. Am. Chem. Soc.* **2016**, *138*, 10323. (g) S. Lukman *et al.*, *J. Am. Chem. Soc.* **2017**, *139*, 18376.

[3] (a) Z. Zeng *et al.*, *J. Am. Chem. Soc.* **2012**, *134*, 14513. (b) Z. Zeng *et al.*, *J. Am. Chem. Soc.* **2013**, *135*, 6363. (c) Z. Zeng *et al.*, *Angew. Chem. Int. Ed.* **2013**, *52*, 8561. (d) Z. Zeng *et al.*, *J. Am. Chem. Soc.* **2015**, *137*, 8572. (e) G. Li *et al.*, *Angew. Chem. Int. Ed.* **2017**, *56*, 5012. (f) H. Zhang *et al.*, *Angew. Chem. Int. Ed.* **2017**, *56*, 13484. (g) J. Wang *et al.*, *Angew. Chem. Int. Ed.* **2017**, *56*, 14154.

[4] (a) P. Hu *et al.*, *J. Am. Chem. Soc.* **2016**, *138*, 1065. (b) S. Das *et al.*, *J. Am. Chem. Soc.* **2016**, *138*, 7782. (c) X. Lu *et al.*, *J. Am. Chem. Soc.* **2016**, *138*, 13048. (d) X. Lu *et al.*, *J. Am. Chem. Soc.* **2017**, *139*, 13173. (e) C. Liu *et al.*, *Chem* **2018**, accepted.

[5] (a) W. Zeng *et al.*, *Chem* **2017**, *2*, 81. (b) Y. Gu *et al.*, *Angew. Chem. Int. Ed.* **2018**, accepted.

[6] (a) X. Gu *et al.*, *Angew. Chem. Int. Ed.* **2017**, *56*, 15383. (b) S. Wu *et al.*, *Angew. Chem. Int. Ed.* **2018**, accepted.

[7] S. Datta *et al.*, *Nat. Commun.* **2017**, *8*, 677.