

# Exploring Novel Nonbenzenoid Hydrocarbons toward Unusual Yet Stable Optoelectronic Materials

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Advancements made to date in organic optoelectronic materials are primarily attributed to aromatic hydrocarbons and their heteroaromatic analogs. These class of compounds are highly valued for their high thermal and chemical stability and desirable properties. They have stimulated the development of various synthetic methodologies, resulting in a wide variety of molecular materials. However, innovative molecular designs and exploration into uncharted chemical spaces are crucial to achieving properties and functionalities beyond the capabilities of existing organic materials. In this context, nonbenzenoid hydrocarbons and related cross-conjugated  $\pi$ -electron systems are an attractive class of compounds due to their characteristic properties such as long-wavelength absorption, multistep redox properties, and distinctive behaviors in excited states, most of which are difficult to attain with benzenoid  $\pi$ -electron systems of comparable molecular weight. Despite their potential, nonbenzenoid  $\pi$ -electron systems remained unexplored as optoelectronic materials due to the difficulty in their synthesis, high reactivity, and a lack of guiding principles for molecular aimed at material applications. Our motivation is to explore the potential of nonbenzenoid  $\pi$ -electron systems as game-changing building blocks for next-generation functional materials, tackling the longstanding issues from three perspectives: to ensure stability without bulky substituents, to develop efficient synthetic methods, and to provide molecular design guidelines to harness their characteristic properties. This presentation will provide an overview of our strategies and some of the recent research along two major topics as follows: (1) Strategy for the stabilization of labile nonbenzenoid  $\pi$ -conjugated systems without using bulky substituents,<sup>1-4</sup> (2) Novel molecular design concepts of electron-accepting hydrocarbons without relying on the electron-withdrawing groups.<sup>5-8</sup>

## References

- 1) (a) A. Fukazawa, H. Oshima, S. Yamaguchi *et al.* *J. Am. Chem. Soc.* **2013**, *135*, 1731. (b) H. Oshima, A. Fukazawa, S. Yamaguchi *et al.* *J. Am. Chem. Soc.* **2014**, *136*, 8738.
- 2) A. Fukazawa, H. Oshima, S. Yamaguchi *et al.* *Angew. Chem. Int. Ed.* **2015**, *54*, 7636.
- 3) (a) J. Usuba, A. Fukazawa *et al.* *Chem. Eur. J.* **2021**, *27*, 1638. (b) J. Usuba, A. Fukazawa, *Chem. Eur. J.* **2021**, *27*, 16127.
- 4) H. Oshima, A. Fukazawa, S. Yamaguchi, *Angew. Chem. Int. Ed.* **2017**, *56*, 3270.
- 5) M. Hayakawa, N. Sunayama, S. I. Takagi, Y. Matsuo, S. Yamaguchi, S. Seki, A. Fukazawa, *Nat. Commun.* **2023**, *14*, 2741.