

CiQUS Lecture



Prof. Michael Haley

UNIVERSITY OF
OREGONRichard M. & Patricia H. Noyes Professor
Department of Chemistry & BiochemistryThe Interplay Between Antiaromaticity
and Diradical Character in Diarenoindacenes
and DiindenoarenesFONDO EUROPEO DE DESENVOLVEMENTO REGIONAL
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Abstract:

This talk will present our synthetic, structural, computational and materials studies of a class of carbon-rich semiconducting molecules based on the indenofluorene (IF) skeleton.¹ Access to the fully conjugated, 20 π -electron, formally antiaromatic system is accomplished via a variety of intermediate diones. These molecules in turn can be assembled via well-known organic possesses (Suzuki cross-coupling, benzylic oxidation, Friedel-Crafts acylation/alkylation).¹ Optimization of their synthesis now permits access to IF derivatives in multigram quantities. We have shown that thin films or single crystals of several different IF scaffolds can serve as an active layer in organic field effect transistors (OFETs).² Current studies (Figure 1) are focused on varying the antiaromaticity of the indacene unit by systematic alteration of the outer benzene groups with other aromatic units³ as well as on increasing the diradical character of the framework by expansion of the quinoidal core.⁴

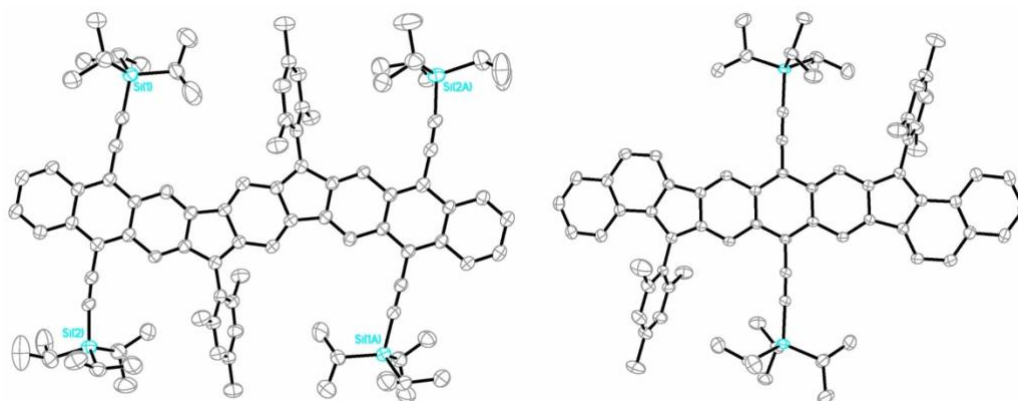


Figure 1. X-ray crystal structures of two π -expanded molecules recently prepared by the Haley group.

Keywords: antiaromaticity • diradical • organic semiconductor • NICS calculations

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2. (a) Marshall et al., *Chem. Sci.* **2016**, *7*, 5547-5558; (b) Zeidell et al., *Chem. Mater.* **2019**, *31*, 6962-6970.
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Biosketch:

Michael M. Haley was born in 1965 in Lake Charles, Louisiana but spent most of his pre-college years growing up in Tulsa, Oklahoma. He received both his Bachelor's (1987) and Ph.D. (1991) degrees from Rice University working with Prof. Ed Billups on the chemistry of cyclopropenes and cycloproparenes. Haley then pursued his postdoctoral studies with Prof. Peter Vollhardt at the University of California-Berkeley from 1991 to 1993 studying [N]phenylenes. He joined the faculty at the University of Oregon in 1993 where he is currently the Richard M. and Patricia H. Noyes Professor of Chemistry. He also served as Head of the Department from 2008 to 2014. Haley is a well-recognized expert in the synthesis and study of aromatic and carbon-rich hydrocarbons with potential applications in materials science. He has co-authored over 230 research articles. Haley was recognized for his innovative hydrocarbon research with the 2021 American Chemical Society George A. Olah Award in Hydrocarbon or Petroleum Chemistry.

Research Group website: <https://haleylab.uoregon.edu/>

Email: haley@uoregon.edu