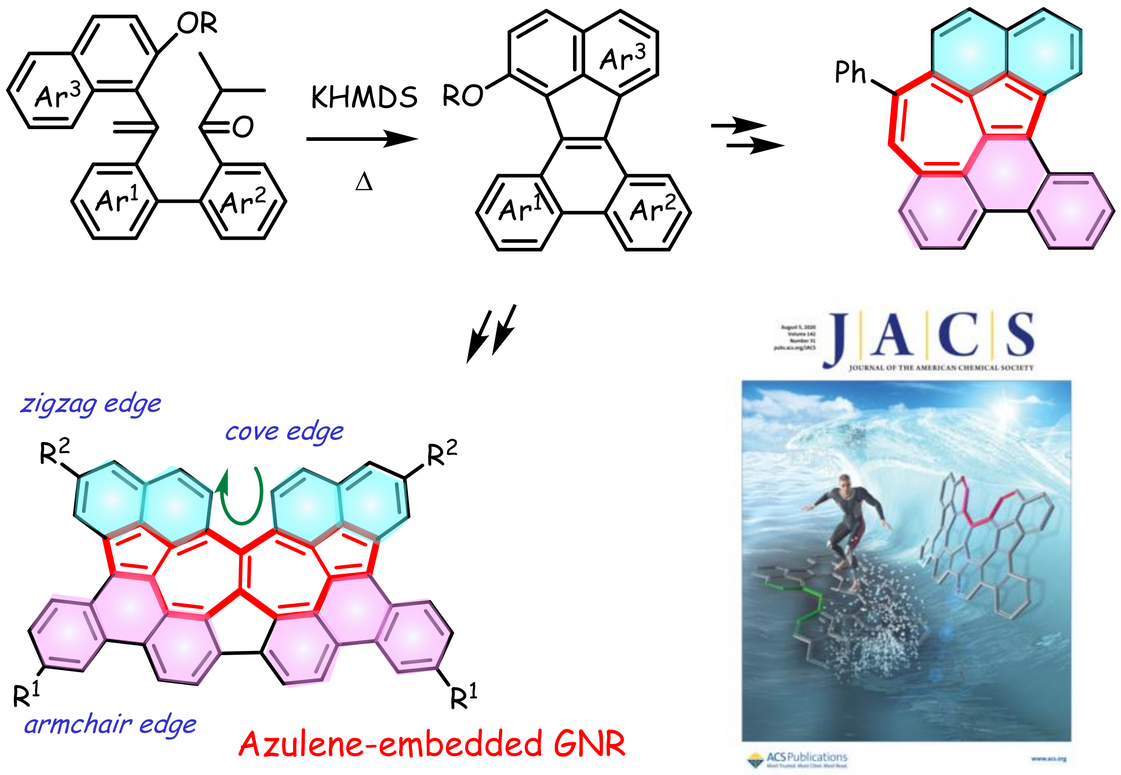
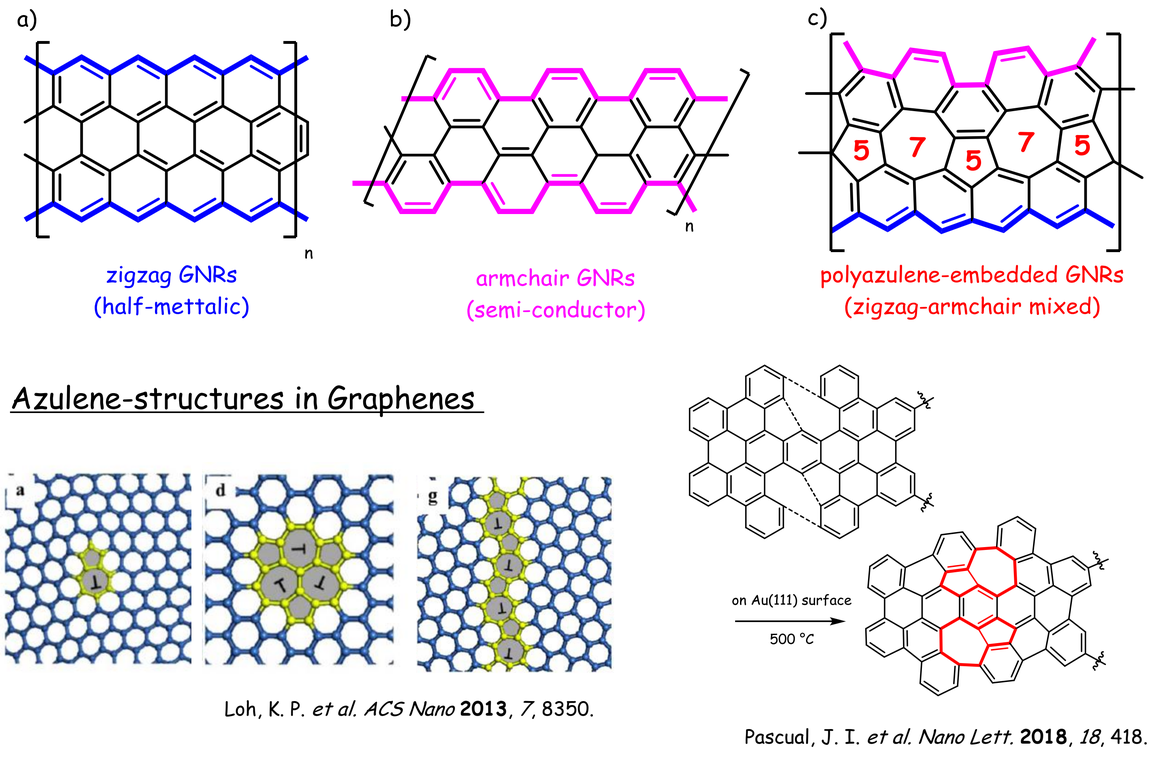
Helical Graphene Nanoribbons Embedded Polyazulene Framework

Naoki Ogawa, Yousuke Yamaoka, Hiroshi Takikawa, and Kiyosei Takasu
(Graduate School of Pharmaceutical Sciences, Kyoto University, Japan)
E-mail: kay-t@pharm.Kyoto-u.ac.jp

1. Abstract



2. Introduction

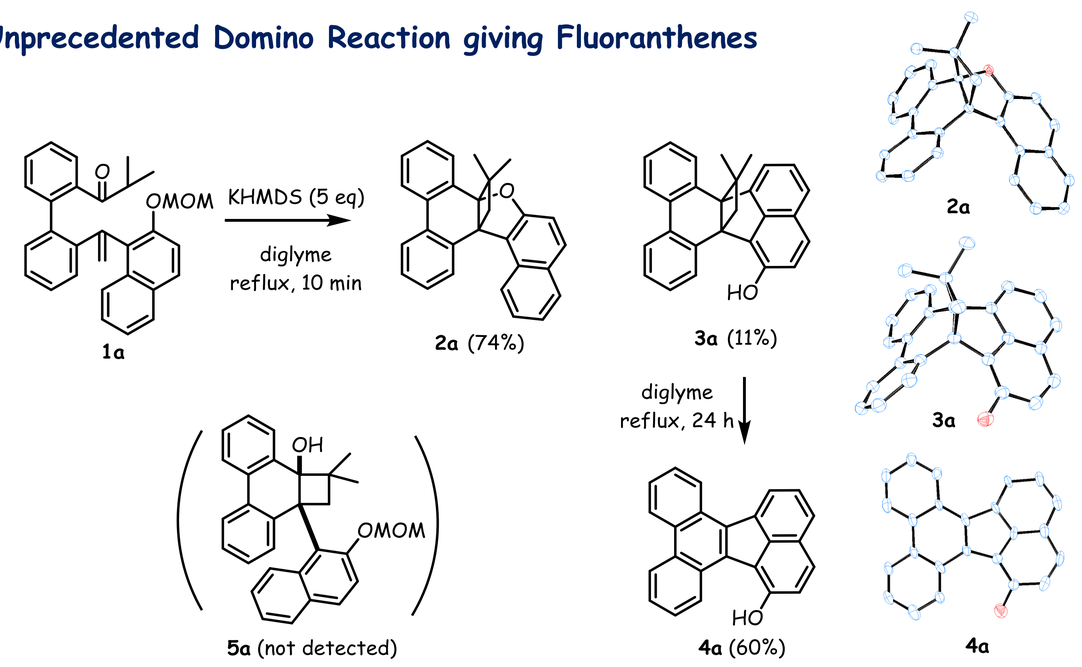


Loh, K. P. *et al. ACS Nano* **2013**, *7*, 8350.

Pascual, J. I. *et al. Nano Lett.* **2018**, *18*, 418.

3. Synthesis of Azuleno-GNRs

Unprecedented Domino Reaction giving Fluoranthenes



Ogawa, N.; Yamaoka, Y.; Yamada, K.; Takasu, K. *Org. Lett.* **2017**, *19*, 3327-3330.

Synthesis of Azulene-embedded Polyaromatic Hydrocarbons

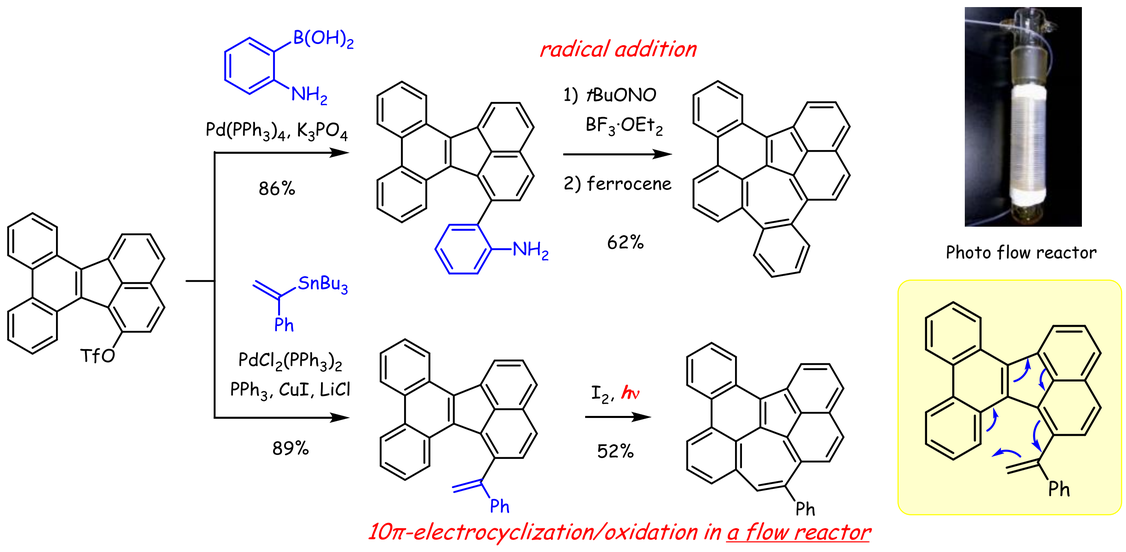
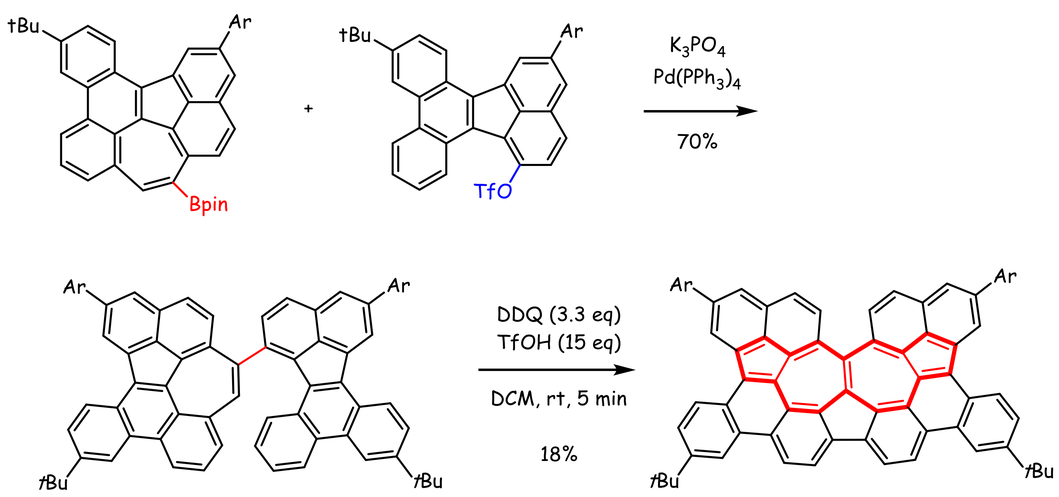


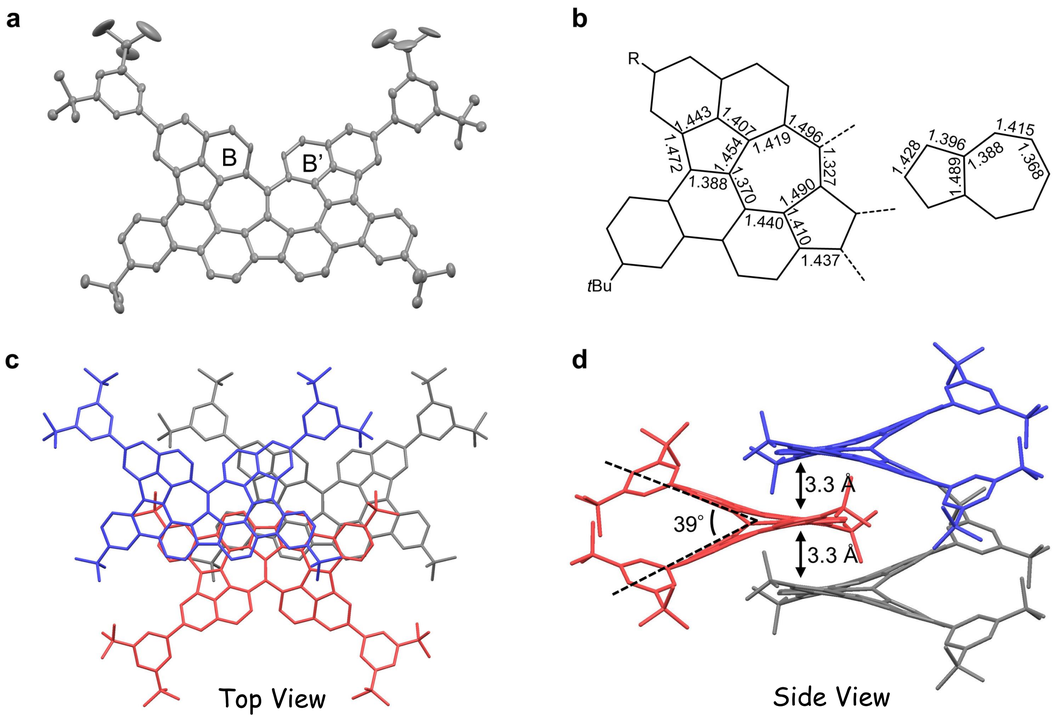
Photo flow reactor

Synthesis of Azulene-embedded GrapheneNanoRibbon

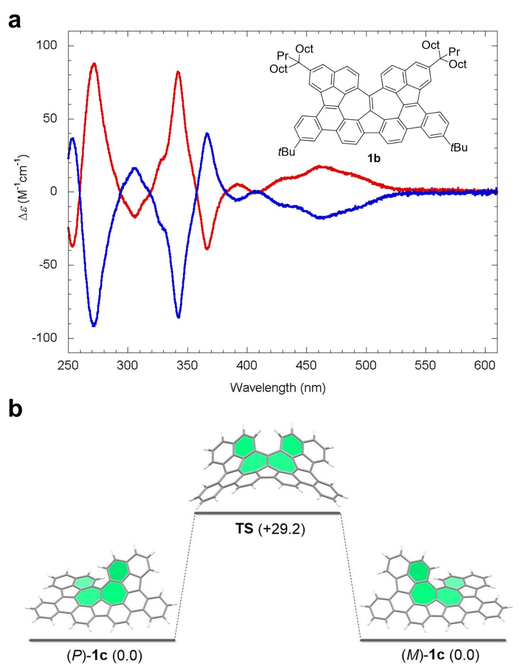


4. Structure of Azuleno-GNR

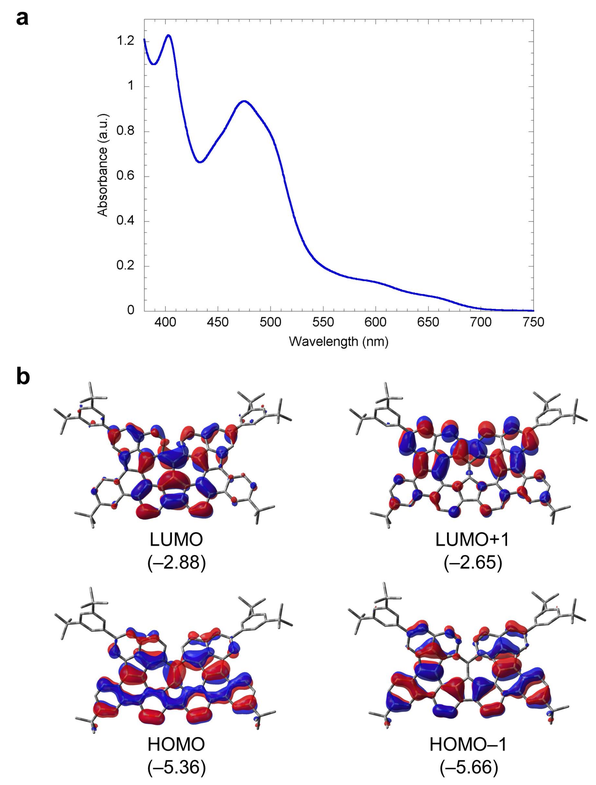
Crystallographic Structure



Molecular Helicity

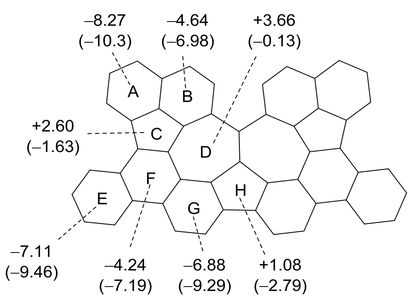


UV-vis & Calculated MO Levels



NICS Values of Azulene-embedded GNR

NICS(0) and NICS(1) values of the model structure (1c). Calculations were conducted at the GIAO-B3LYP/6-311+G(2d,p) theoretical level. NICS(1) values are given in parentheses.



Ogawa, N.; Yamaoka, Y.; Takikawa, H.; Yamada, K.; Takasu, K. *J. Am. Chem. Soc.* **2020**, *142*, 13322-13327.

Supported by MEXT KAKENHI (Middle Molecular Strategy)