

## メカノケミカル水素化による周辺水素化ナノグラフェンの合成と性質

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Mechanochemical arene hydrogenation toward synthesis of periphery-hydrogenated nanographenes and those properties

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Peripherally hydrogenated nanographenes are anticipated to display favorable properties including enhanced solubility and negative electron affinity compared to those mother molecules. However, the synthesis of these molecules generally requires long reaction time under harsh conditions such as high-pressure hydrogenation and high temperature, and the reaction often are suffered from the low solubility of nanographenes. These issues have presented a significant challenge to the synthesis of peripherally hydrogenated nanographene.

Herein, we developed a new approach utilizing rhodium-catalyzed mechanochemical hydrogenation, which enables hydrogenation without the use of hydrogen gas. In the presentation, we will present the rapid synthesis of various peripherally hydrogenated nanographenes by this method as well as substrate scope and their unique physical properties.

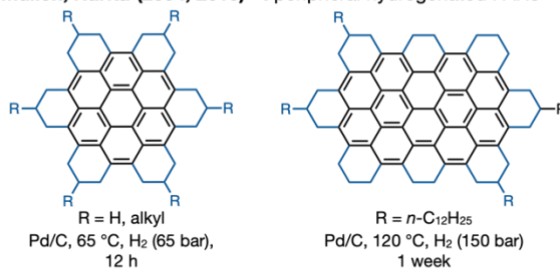
**Keywords:** Mechanochemical reaction, Ball-milling, Polycyclic Aromatic Hydrocarbons (PAHs), Hydrogenation, Hydrogenated nanographene

周辺水素化ナノグラフェンは、高い溶解性や負の電子親和力など、好ましい性質を示すことが期待される分子群である<sup>[1,2]</sup>。しかし、これらの分子群の合成には、一般的に高圧水素化処理に長時間を要すること、出発原料であるナノグラフェンの溶解度が極めて低いことが課題となっており、合成難易度を高めていた。

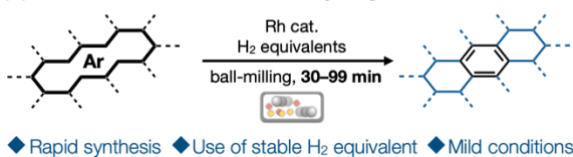
今回我々は、ロジウム触媒を用いたメカノケミカル水素化反応により、水素ガスを用いずに水素化できる新しい合成アプローチを開発した。水素源として無機塩を用い<sup>[3]</sup>、系中で水素等価体を発生させることで低溶解性のナノグラフェンの迅速水素化に成功した。発表では、この方法による様々な周辺水素化ナノグラフェンの迅速合成、基質範囲、およびそれらのユニークな物性について紹介する。

### (A) Hydrogenated nanographenes

Müllen, Narita (2004, 2019)<sup>1,2</sup>: peripheral hydrogenated PAHs



### (B) This work: Mechanochemical hydrogenation of arenes



[1] M. D. Watson, M. G. Debije, J. M. Warman, K. Müllen, *J. Am. Chem. Soc.* **2004**, 126, 766.

[2] X. Yao, X. Y. Wang, C. Simpson, G. M. Paternò, M. Guizzardi, M. Wagner, G. Cerullo, F. Scotognella, M. D. Watson, A. Narita, K. Müllen, *J. Am. Chem. Soc.* **2019**, 141, 4230.

[3] Y. Wang, Z. Chang, Y. Hu, X. Lin, X. Dou, *Org. Lett.* **2021**, 23, 1910.