

バーチャル配位子法を用いたインシリコ配位子設計法の開発と末端イナミドのヒドロゲルミル化反応への応用

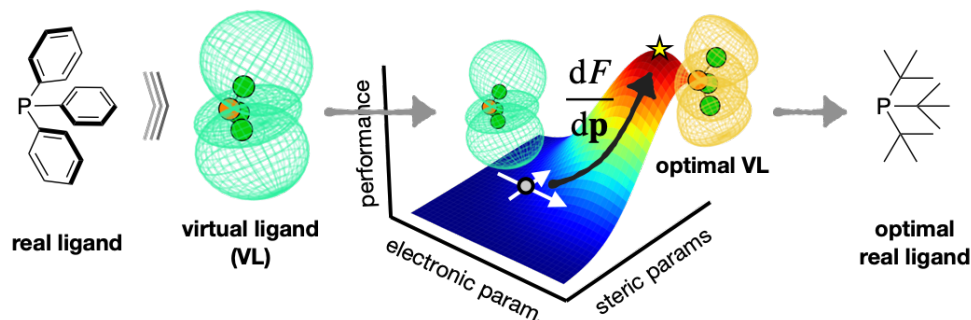
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Development of Virtual Ligand-Assisted Optimization Method for *In Silico* Ligand Engineering and Its Application to Hydrogermylation of Terminal Ynamide (¹WPI-ICReDD, Hokkaido University, ²JST-ERATO, ³Faculty of Science, Hokkaido University, ⁴Graduate School of Chemical Sciences and Engineering, Hokkaido University, ⁵Graduate School of Information Science and Technology, The University of Tokyo, ⁶University of Bristol, ⁷University of Oxford) ○Wataru Matsuoka,^{1,2,3} Taihei Oki,^{1,2} Ren Yamada,⁴ Tomohiko Yokoyama,⁵ Shinichi Suda,⁴ Carla M. Saunders,⁶ Bastian Bjerkem Skjelstad,⁷ Yu Harabuchi,^{1,2} Satoru Iwata,^{1,2,5} Satoshi Maeda^{1,2,3}

Ligand engineering is one of the most important, but labor-intensive processes in the development of transition metal catalysis. Herein, we report the virtual ligand-assisted optimization (VLAO) method, a fundamentally new *in silico* approach for ligand engineering. In this method, the virtual ligand, a dummy ligand for quantum chemical calculations, is used to identify important electronic and steric features for ligand engineering. We demonstrated the VLAO calculation for the α -selective hydrogermylation of a terminal ynamide, and ideal ligand features were automatically identified. In the presentation, the theory behind the VLAO method will be briefly explained, followed by the results of its application to actual ligand design.

Keywords : *In Silico Catalyst Optimization; Virtual Ligand; Quantum Chemical Calculation*

遷移金属触媒の設計には、多数の配位子候補からいかに効率的に最適配位子を選択できるかが極めて重要である。我々は、量子化学計算と簡単な数学的操作により目的の反応に最適な触媒の特徴を見出すバーチャル配位子アシスト最適化(VLAO)法を開発した。本手法をもとに量子化学計算に基づいて触媒設計指針を定めることで、迅速かつ合理的に最適触媒を見出すことが可能である。発表では VLAO 法の詳細と末端イナミドのヒドロゲルミル化反応に適用した結果を述べる。



1) Matsuoka, W.; Oki, T.; Yamada, R.; Yokoyama, T.; Suda, S.; Saunders, C. M.; Skjelstad, B. B.; Harabuchi, Y.; Fey, N.; Iwata, S.; Maeda, S. *ACS Catal.* **2024**, *14*, 16297.