Applications of ab initio methods in transition metal chemistry: from qualitative description to quantitative spin state

Quan Manh Phung[†,‡]

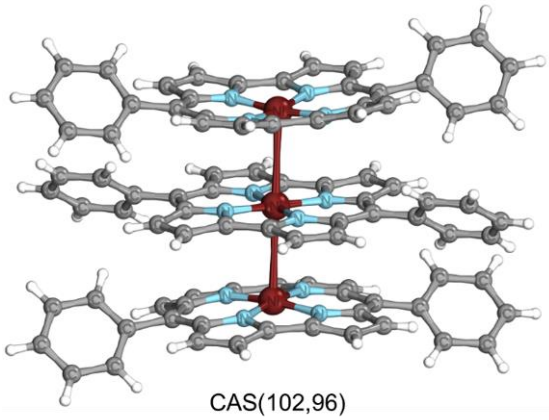
†*Department of Chemistry, Graduate School of Science, Nagoya University, Furo-cho, Chikusa-ku, Nagoya, Aichi, 464-8602, Japan*

‡*Institute of Transformative Bio-Molecules (WPI-ITbM), Nagoya University, Furo-cho, Chikusa-ku, Nagoya, Aichi, 464-8602, Japan*

E-mail: quan.phung@chem.nagoya-u.ac.jp

Abstract

Ab initio methods have nowadays adopted a crucial collaborative role with experiments in exploring the properties and reactivity of transition metal (TM) compounds. In this talk, we discuss recent advancements in ab initio methods to study TM compounds. We demonstrate the applicability of these novel methods, especially the density matrix renormalization group (DMRG)-based techniques, in a wide range of mono-, bi-, and tri-nuclear TM containing systems: from a qualitative description of metal-corrole complexes to quantitative characterization of the spin-state energetics of iron porphyrin derivatives and the C-H activation of ultrahigh-valent diiron–oxo species.[1–3]



CAS(102,96)

[1] K. Pierloot, Q. M. Phung, A. Ghosh, *Inorg. Chem.* **2020**, *59*, 11493–11502.

[2] Q. M. Phung, Y. Muchammad, T. Yanai, A. Ghosh, *JACS Au* **2021**, *1*, 2303–2314.

[3] Q. M. Phung, K. Pierloot, *Chem. – A Eur. J.* **2019**, *25*, 12491–12496.