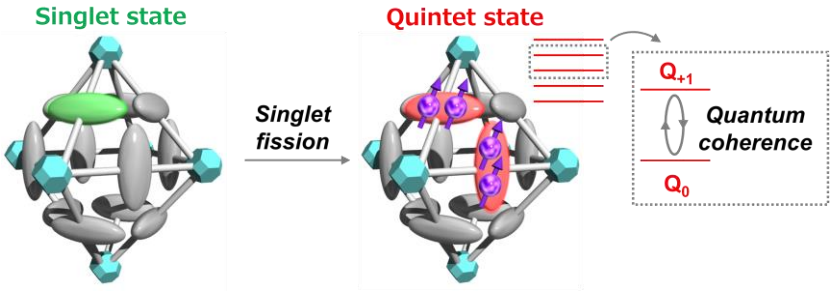
Room-temperature quantum coherence of quintet state generated through singlet fission in a metal-organic framework

([1]*Kyushu University*, [2]*Kobe University*, [3]*CREST, JST*, [4]*RIKEN*, [5]*FOREST, JST*) ○Akio Yamauchi,[1] Kentaro Tanaka,[1] Masaaki Fuki,[2,3] Saiya Fujiwara,[4] Nobuo Kimizuka,[1] Tomohiro Ryu,[1] Masaki Saigo,[1] Ken Onda,[1] Ryota Kusumoto,[2] Nami Ueno,[2] Harumi Sato,[2] Yasuhiro Kobori,[2,3] Kiyoshi Miyata,[1,3] Nobuhiro Yanai[1,3,5]

Keywords: Singlet fission; Quintet state; Qubit; Quantum coherence; Metal-organic framework

A quantum bit (qubit) that expands a concept of bit to a two-level quantum state, is a basic building block of quantum information science to realize quantum technologies such as quantum computing and quantum sensing.[1] Qubits based on electron spins of molecules has several advantages such as a high controllability of qubit properties by chemical modifications. Among the molecular qubit, quintet state generated through singlet fission (SF) has unique feature of being consisted by four spins, which enables advanced qubit operations.[2] To utilize the quintet state as a qubit, the generation of the quantum spin coherence in the quintet sublevels are required. However, there were no reports about the quantum coherence at room temperature.

Here we reports the first observation of the room-temperature quantum coherence of the quintet state generated though SF in a metal-organic framework (MOF).[3] A typical SF molecule, pentacene was modified and loaded as the ligand. The existence of SF and the quintet state in the MOF (Pn-MOF) was confirmed by transient absorption spectroscopy and time-resolved electron paramagnetic resonance (EPR). Nutation measurement with pulsed EPR shows the quantum coherence of the quintet state. The simulation based on the results indicate the suppressed motion in the densely packed MOF contributes the generation of the quintet state with keeping its quantum coherence.



1) C. L. Degen, F. Reinhard, P. Cappellaro *Rev. Mod. Phys*. **2017**, *89*, 035002. 2) R. M. Jacobberger, Y. Qiu, M. L. Williams, M. D. Krzyaniak, M. R. Wasielewski, *J. Am., Chem. Soc*. **2022**, *144*, 2276. 3) A. Yamauchi et al., *Sci. Adv.* **2024**, *10*, eadi3147.

© The Chemical Society of Japan