

Ortho-para nuclear spin isomer fluctuation of a H₂O molecule in H₂O@C₆₀ single molecule transistors

H₂O@C₆₀ 単一分子トランジスタ中の水分子のオルソ-パラ核スピン異性体間揺らぎ

¹東大生研・²ナノ量子機構・³上海マイクロシステム情報技術研、⁴京大化研、⁵東北大理
田 玥¹, 杜 少卿^{1,3}, 橋本克之⁵, 橋川祥史⁴, 村田靖次郎⁴, 平山祥郎⁵, 平川一彦^{1,2}

¹IIS/INQIE, Univ. of Tokyo, ³SIMIT, CAS, ⁴ICR, Kyoto Univ., ⁵Phys. Dept., Tohoku Univ.

°Yue Tian¹, Shaoqing Du³, Katsushi Hashimoto⁵, Yoshifumi Hashikawa⁴, Yasujiro Murata⁴, Yoshiro Hirayama⁵,
Kazuhiko Hirakawa^{1,2}

E-mail: tianyue@iis.u-tokyo.ac.jp

The nuclear spin isomers of a H₂O molecule in single H₂O@C₆₀ molecule, in which a single water molecule is encapsulated within a C₆₀ fullerene cage, is attractive for its potential applications to quantum memory. In our previous study, we performed tunneling spectroscopy measurements on H₂O@C₆₀ single molecule transistors (SMTs) and observed both para (p)- and ortho (o)-states in tunneling conductance spectra, which suggests that the nuclear spin state of H atoms in the H₂O molecule fluctuates quickly between the p-and o-states [1]. However, systematic investigation on how this o-p fluctuation takes place is still missing.

We propose a "selection rule" for the o-p conversion process in H₂O@C₆₀ SMTs. Figures 1(a), 1(c), and 1(e) show energy diagrams, illustrating possible nuclear spin flip processes. The angular momentum of the system consists of rotational excitation of the H₂O molecule (J), spin of a conduction electron (S), and the nuclear spin (I). During the tunneling process, total angular momentum $F = I+J+S$ needs to be conserved. Figures 1(a), 1(c), and 1(e) respectively illustrate the interactions between I and S , between I and J , and of all I , J , and S . Diagonal transition paths generate different excited states that appear in the Coulomb stability diagrams, shown in Figures 1(b), (d), and (f). Details will be discussed in the presentation.

References [1] S. Du et al., Nano Lett. **21**, 24 (2021).

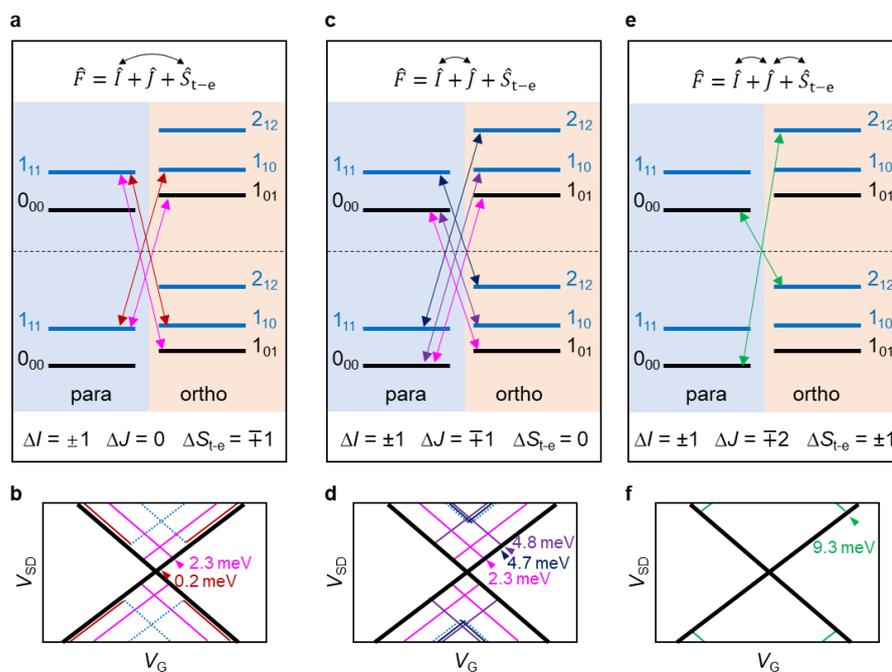


Fig.1 Possible conversion processes between o-H₂O and p-H₂O, involving (a) spin of a conduction electron, (c) rotational excitation of H₂O molecule, and (e) both electron spin and molecule rotation. The corresponding Coulomb stability diagrams are shown in (b), (d), and (f).