Quantum entanglement state between photoelectron spin and emitted X-ray photon polarization in spin and polarization resolved XEPECS of Ti_2O_3

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➢ R. B. Tanaka et al., J. Phys. Soc. Jpn. **94**, 104402 (2025).

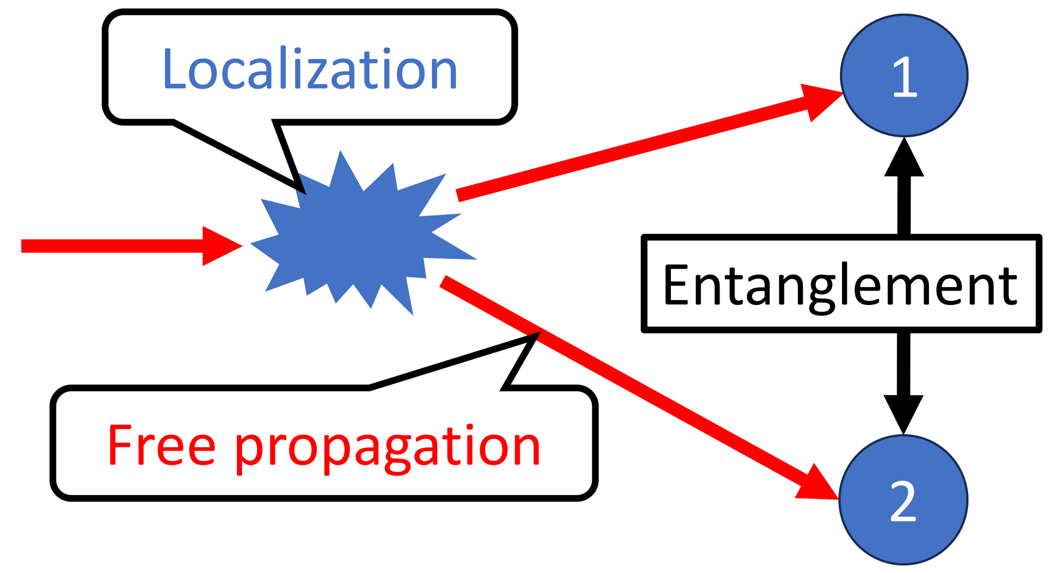
Introduction

Quantum entanglement

➢ A. Aspect et al., Phys. Rev. Lett. **47**, 460 (1981).

Quantum entanglement is a phenomenon where the quantum state of each particle cannot be described independently of the state.
→ "Localization" and "Free propagation" are required

Entangled state : $|\psi\rangle \neq |\psi\rangle_1 \otimes |\psi\rangle_2$

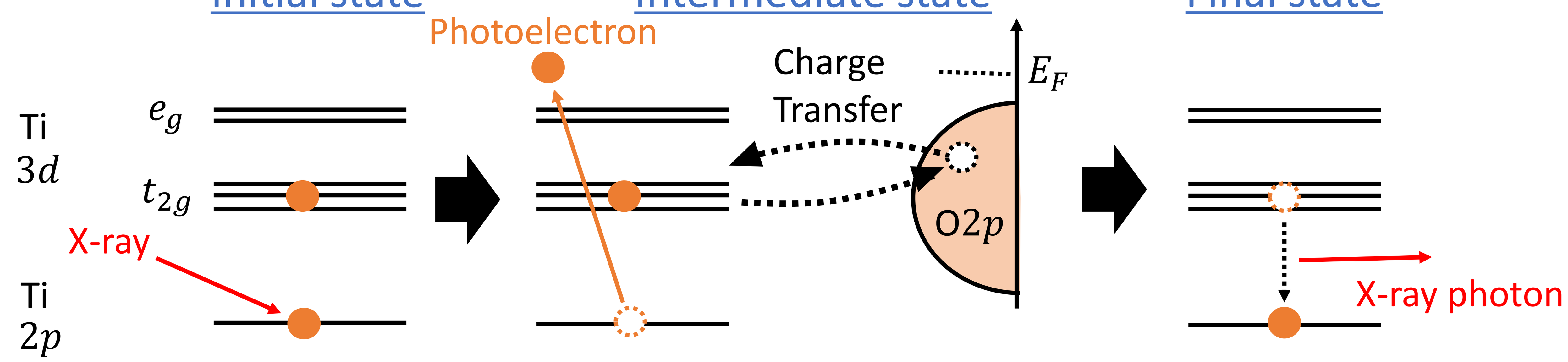


The hypothesis of this study

We hypothesize that the photoelectron and the emitted X-ray photon generated by X-ray inner-shell excitation form a quantum-entangled state, because two key conditions for entanglement are satisfied.

- Localization:
  The core-hole potential strongly confines local electron interactions.
- Free propagation:
  Both the photoelectron and X-ray photon are emitted with high energy and escape from the material almost instantaneously.

Method 1 : $3d \rightarrow 2p$ XEPECS process for Ti_2O_3

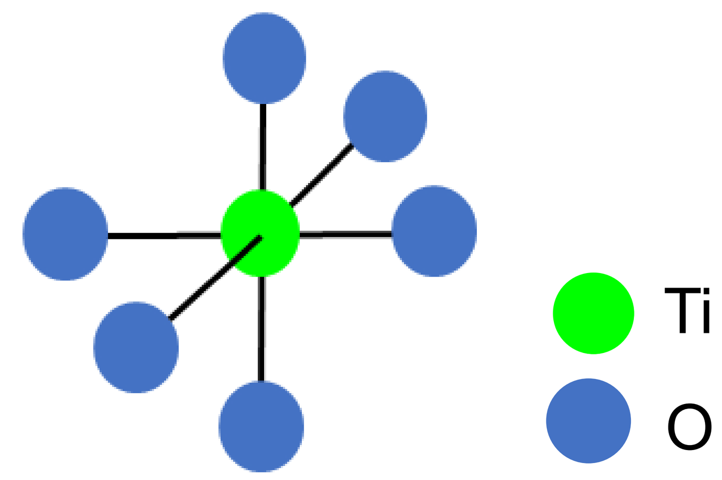


Purpose of this poster

- For Ti_2O_3, we demonstrate the generation of the spin and polarization entanglement in the $3d \rightarrow 2p$ XEPECS process.
- We clarify how the entanglement depends on both charge-transfer and crystal field.

Method 2 : TiO_6-type cluster model

■ TiO_6-type cluster model for Ti_2O_3

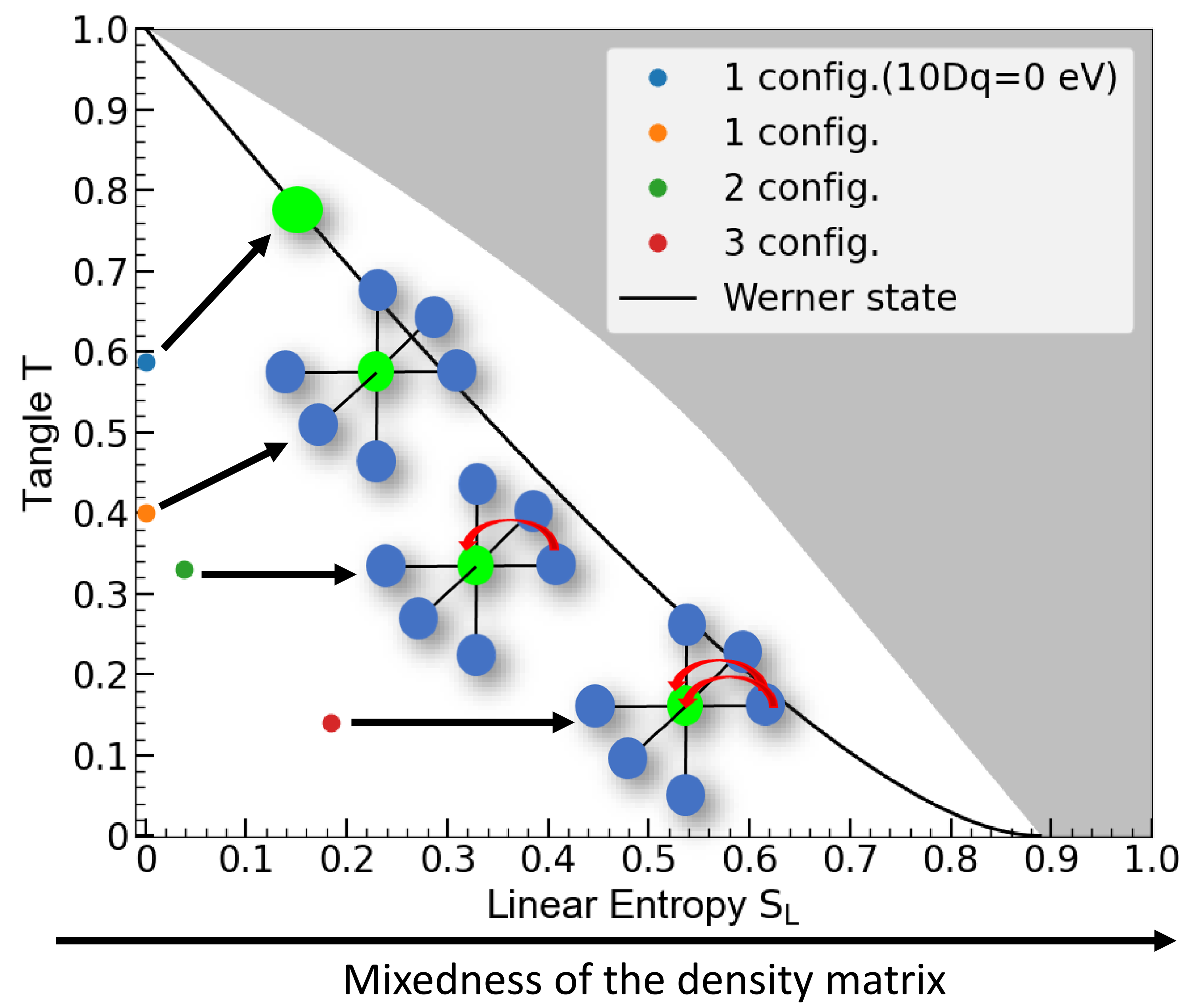


■ Solid-state parameters (eV)

- Charge-transfer energy : $\Delta = \epsilon_d - \epsilon_L$
- Ti $3d$ – O $2p$ hybridization : $V(e_g)$
- Ti $3d$ crystal-field splitting : $10Dq$
- $d-d$ Coulomb interaction : U_{dd}
- Core-hole potential : U_{dc}

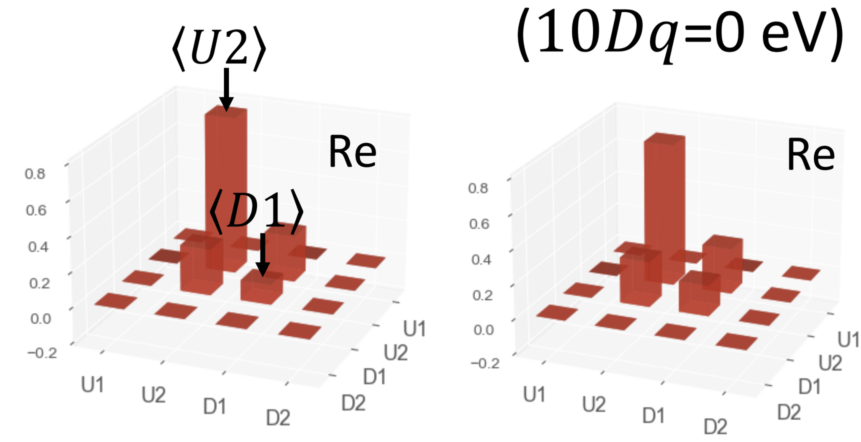
Result : Effects of Ti–O Hybridization and Crystal Field on the Entangelement

■ Relationship between tangle and linear entropy



■ Crystal-field effect

@ 1config. @ 1config. ($10Dq$=0 eV)



$10Dq$ (eV)	$\langle U2\rangle - \langle D1\rangle$
0.5	0.77
0.0	0.64

Crystal field effect
↓
larger difference between diagonal elements
↓
weaker entanglement

Messages

- The hybridization effect disturbs the localized state in a single atom, resulting in a decrease of the tangle.
- The crystal-field effect also decrease the tangle due to the asymmetry of the diagonal elements in the density matrix.