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Ground state instability in spin polarization for electrons confined in 2D square quantum dots KYOZABURO TAKEDA, MASAMU ISHIZUKI, TAKUMA OKUNISHI, YHUKI NEGISHI, Waseda University — We present a theoretical study of the ground state electronic structure and the spin polarization for four electrons confined in 2D square quantum dots (2D SQDs). We employ standard mean field theory (MFT) approaches using the unrestricted Hartree-Fock (UHF) and density functional theory (DFT) calculations. The resonant UHF configuration interaction (res-UHF CI) calculation was also performed in order to understand the electron correlation more intuitively. The MFT ground state is expected to be fully spin-polarized when square SQDs have a small confinement length L or aspect ratio, in agreement with Hund's rule. In contrast, the spin-unpolarized ground state singlet is expected in all in other SQDs, the MFT anti-Hund state is produced by the spin-density wave having the zero total spin. The res-UHF CI calculation restores the geometrical symmetry in the resulting ground state, but the res- UHF CI ground state maintains the zero total spin. Thus, ground state instability is expected in the spin-polarization of the SQD system, which eventually violates Hund's rule in accordance with the Coulomb interaction.

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