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Interpretation of Hund's multiplicity rule for the atomic systems KENTA HONGO, TAKAYUKI OYAMADA, Institute for Materials Research, Tohoku University, RYO MAEZONO[1], National Institute for Materials Science, YOSHIYUKI KAWAZOE, HIROSHI YASUHARA, Institute for Materials Research, Tohoku University, M.D. TOWLER, R.J. NEEDS, TCM Group, Cavendish Laboratory, University of Cambridge — We have studied Hund's multiplicity rule for the carbon atom using quantum Monte Carlo methods[1]. Our calculations give a high-level description of electron correlation and satisfy the virial theorem to high accuracy. This allows us to obtain accurate and reliable values for each of the energy terms and therefore to give a convincing explanation of the mechanism by which Hund's rule operates in carbon. We obtain the following results: (1) the energy gain in the triplet with respect to the singlet state is due to the greater electron-nucleus attraction in the higher spin state, and (2) the electron-electron repulsion in the triplet is greater than that in the singlet, in accordance with Hartree-Fock results and studies including correlation. Although our main topic is the carbon atom, we would also like to show our current results of the nitrogen atom.[1]K. Hongo, *et al.*, J. Chem. Phys. **121**, 7144 (2004).

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