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Understanding of Nuclear Quadrupole Interaction of ^{19}F* and Binding Mechanism in Solid Fluorine at First-Principles Level D.R. MISHRA, M.M. ARYAL, N.P. ADHIKARI, Central Department of Physics, Tribhuvan University, Kirtipur, Kathmandu, Nepal, R.H. PINK, T.P. DAS, Department of Physics, University at Albany, SUNY — We have carried out a theoretical study of the nuclear quadrupole interaction (NQI) parameters of ^{19}F* excited nuclear state in solid fluorine as well as the intermolecular binding of fluorine molecules in the solid. This is in continuation of our investigation [1] of the properties of solid halogens using the first-principles Hartree-Fock (HF) cluster procedure combined with many-body perturbation theory (MBPT), implemented by the Gaussian 03 set of programs. For the NQI parameters, the value of (e^2qQ/h) obtained from our investigation for the ^{19}F* excited nuclear state in solid fluorine is 120.9 MHz, which agrees with the experimental value 127.2 MHz, quoted in [2], within 5% and the asymmetry parameter, η is essentially zero. For obtaining (e^2qQ/h) the value of the quadrupole moment, Q for ^{19}F* is taken from [3] as 0.072 x 10^{28} m^2. As regards the binding of fluorine molecules in solid fluorine, our quantitative binding energy results show that the binding arises mainly from the van der Waals interaction obtained from intermolecular many-body effects with the one electron HF contribution being weak and repulsive in nature.

[1] M.M. Aryal et al., Hyperfine Interact, 176, 51 (2007).
[2] K.C.Mishra et al.,Phys. Rev.B25, 3389(1982).
[3] H. Barfuss et al., Phys. Lett. 90A, 33(1982).

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