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First-Principles Study of Nuclear Quadruple Interaction of ^{19}F* and Binding in Solid Fluorine D.R. MISHRA, M.M. ARYAL, N.P. ADHIKARI, TU Kirtipur, Kathmandu, Nepal, S.R. BADU, R.H. PINK, SUNY Albany, R.H. SCHEICHER, Uppsala University, Sweden, LEE CHOW, UCF Orlando, T.P. DAS, SUNY Albany — We have studied the binding energy (BE) and nuclear quadrupule interaction (NQI) parameters for the ^{19}F* excited nuclear state in solid fluorine as part of our investigation [1] of the properties of solid halogens using the first principles Hartree-Fock Cluster procedure combined with many-body perturbation theory (MBPT), implemented by the Gaussian set of programs. Our results show that Van der Waals interaction obtained from intermolecular electron correlation effects has dominant influence on the BE but negligible effect on the NQI parameters. For the latter, ourcalculated e^2qQ is 119.0MHz using for Q(19F*), the value of 0.072 $*10^{-28}$m2 [2], and η, the asymmetry parameter, is essentially zero. The influence of rotational vibrational effects on e^2qQ is being investigated using a first-principles procedure [3] to bridge the small remaining difference with experiment (127.2 MHz) for e^2qQ [4]. [1] M.M. Aryal et al., Hyperfine Interact, 176, 51 (2007). [2] K.C.Mishra et al.,Phys. Rev.B25, 3389(1982). [3] N. Sahoo et al. Phys. Rev. Lett. 50, 913(1983) [4] H. Barfuss et al., Phys. Lett. 90A, 33(1982)

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