AB INITIO STUDY OF NEUTRAL AND IONIC FeS_n CLUSTERS

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Iron-Sulphur clusters in various iron sulphur proteins play diverse biological functions. Computational study of these complexes are challenging due to the close-lying states of multi-reference charactor. We carried out extensive CASSCF followed by MRCI calculations using the relativistic all-electron Douglas-Kroll approach. We also carried out QMC calculations using the CASINO pseudopotential and basis function optimized with it. New features in the CHAMP QMC package allow us to optimize the expansion coefficients of the multi-determinant trial wavefunction as well as the linear combination coefficients of the orbitals and the exponents of the basis functions used to construct the trial wavefunction. Calculated results are compared with available experimental results.