Scientific Achievement

The relative spin-state and binding energies of FeF$_2$···C$_2$H$_6$, and FeF$_2$···C$_2$H$_4$, along with the relative spin-state energies of FeF$_2$ with respect to the quintet ground spin state, were investigated using both single-configurational and multiconfigurational methods, giving new benchmarks.

Significance and Impact

The variance in performance of different functionals in describing relative-spin state energies shows that one must be extra cautious to consider a sufficiently flexible open-shell solution and all possible electronic configurations when carrying out electronic structure calculations on open-shell transition-metal systems.

Research Details

The performance of both single-configurational methods (Hartree–Fock method, 32 exchange–correlation functionals, and the CCSD(T) coupled-cluster method in both restricted and unrestricted formalisms) and multiconfigurational methods (CASSCF, CASPT2, CASPT3, MRCI, MRCI+Q, and MR-ACPF) on FeF$_2$, FeF$_2$···C$_2$H$_6$, and FeF$_2$···C$_2$H$_4$ were studied.