

Coupled Cluster for Lanthanide Monofluorides

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The special properties of lanthanides make them promising for future applications. One of these attributes is the large magnetic moment stemming from the open f-shells resulting in strong magnetism of certain lanthanide based alloys. Another potential application, single molecule magnets, has gained interest in recent years[1]. The f-shells are quite compact and only weakly perturbed by the environment. Consequently, the optical transition involving these molecules only show minor influence of the environment. This is applied in laser crystals and also opens the path for exciting medical applications[2].

In this work we are taking a closer look at lanthanide monofluorides. On one side this has the advantage of only one internal coordinate. On the other side an oxidation state of +1 has a more complex orbital structure, than the more common oxidation states of +2 and +3. In a first step the potential energy curves were computed on the Hartree-Fock level using the average of configuration approach[3] and effective core potentials. We applied the core potentials developed by Dolg *et. al* for this oxidation state[4]. Based on this coupled cluster computation were performed using the DIRAC software package[5] and will be compared to available experimental and theoretical data.

References

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