Consideration of heavy Elements in DFTB – A scalar-relativistic approach

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The interest in investigations of compounds containing heavier elements like e.g. endohedral rare earth fullerenes implies the necessity of the consideration of relativistic effects.

A full solution of the relativistically generalized Kohn-Sham equations would greatly increase the computational effort compared to a non-relativistic treatment. A scalar-relativistic treatment is computationally as fast as a non-relativistic scheme, but considers all relativistic shift effects, direct (Darwin term, mass-velocity term) as well as indirect effects (via potential), only spin-orbit coupling is omitted.

A semirelativistic formulation of the Density-Functional based Tight binding (DF-TB) scheme is proposed. The method is realized within the standard DF-TB implementation without any additional computational effort. All relativistic shift effects are included in the precalculated Hamilton–Matrixelements.

As an application the valence state of rare earth metals in various fullerene cages (e.g. C_{72}, C_{80}, C_{82}, C_{84}) as endohedral complexes were investigated and molecular dynamics simulations on the mobility of rare earth metals in the fullerene cages were studied.