

**Recent developments of two-component relativistic methods
based
on the quaternion modified Dirac equation**

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We present developments of two-component relativistic methods based on the Barysz-Sadlej-Snijders transformation of the quaternion modified Dirac operator in a finite basis set [1].

First, we show that further improvement of the Hamiltonian is possible by extending it with the one-centre mean-field spin-orbit operator. This mean-field screened infinite-order two-component (MFSO-IOTC) Hamiltonian gives best results of properties determined mainly by spin-orbit relativistic effects.

Second, it is possible to perform the same block-diagonalizing transformation of the converged Fock-Dirac operator and continue molecular spinor transformations and correlated calculations upon two-component spinors.

[1] H.J.Aa. Jensen, M.Ilias,

"Two-component relativistic methods based on the quaternion modified Dirac equation. I: from Douglas-Kroll-Hess second order method to the infinite order two-component method", in preparation.