Magnetic anisotropy of homonuclear transition metal dimers

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9.7 cm

Calculated structural and magnetic properties of transition metal dimers are reported. All calculations have been performed using the full-potential local-orbital program package FPLO [1] for the solution of the Kohn-Sham-Dirac equations within the local spin density approximation (LSDA). The structural properties, such as ground state spin multiplicity, bond length, and harmonic vibrational frequency, are obtained by scalar-relativistic calculations. The fixed-spin moment method is applied to stabilise the convergence and to single out the ground state spin state. In the next step, orbital magnetic properties are obtained from spin polarised full-relativistic calculations. Since orbital moments are usually underestimated in such calculations, we have additionally studied the influence of orbital polarisation corrections (OPC, [2]). The results will be compared with available experimental data and other theoretical investigations.

[1] K. Koepernik and H. Eschrig, Phys. Rev. B **59**, 1743 (1999); http://www.fplo.de.
[2] L. Nordström, M. S. S. Brooks, and B. Johansson, J. Phys.: Condens. Matter **4**, 3261 (1992).

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