DMRG approach to a molecular-based bimetallic chain containing Re(IV) and CU(II) ions.

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Rok wydania

2010

Czasopismo

Acta Physica Polonica A

Numer woluminu

118

Strony

975-977

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The bimetallic chain complex [Cu(tren)]ReCl_6 is numerically analysed on the basis of the anisotropic quantum Heisenberg model without the mean-field corrections by the density-matrix renormalization group approach. The high accuracy results of our simulations have been fitted to the corresponding experimental susceptibility data above the crossover regime. The set of model parameters comprising the strength of antiferromagnetic couplings, the single-ion anisotropy term and the corresponding g factors have been found: J/k_{B} = 3.5 ± 0.5 K, D/k_{B} = 35 ± 5 K, g_{Cu} = 2.07 ± 0.05 and g_{Re} = 1.73 ± 0.01.

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