

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

Autorzy

P. Sobczak
A. Barasiński
R. Matysiak
A. Drzewiński
Grzegorz Kamieniarz
Alina Bieńko
Jerzy Mroziński

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Streszczenie

The bimetallic chain complex $[\text{Cu}(\text{tren})]\text{ReCl}_6$ 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: $J/k_{\text{B}} = 3.5 \pm 0.5$ K, $D/k_{\text{B}} = 35 \pm 5$ K, $g_{\text{Cu}} = 2.07 \pm 0.05$ and $g_{\text{Re}} = 1.73 \pm 0.01$.

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