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Spin dynamics and quantum states in 3d atomic chains on Cu3N-Cu(110) molecular network OLEG STEPANYUK, Max-Planck-Institut für Mikrostrukturphysik; Lomonosov Moscow State University; Russian Academy of Sciences Dorodnicyn Computing Centre of RAS, DMITRY BAZHANOV, Max-Planck-Institut für Mikrostrukturphysik; Lomonosov Moscow State University, VALERI STEPANYUK, Max-Planck-Institut für Mikrostrukturphysik — Based on first-principle calculations we studied the magnetic state and exchange coupling of transition metal atomic chains of Mn, Fe and Co deposited on a self-corrugated Cu3N-Cu(110) molecular network. We considered various atomic sites for adsorption on the corrugated Cu3N layer. By calculating the ground state magnetic configurations it was shown, that the magnetic order, anisotropy and exchange coupling within atomic chains depend sensitively on their chemical composition and adsorption sites on Cu3N network. We have found that exchange coupling in nanowires could be ferromagnetic and anti-ferromagnetic depending on the position of the chain on the surface. The spin-dynamics is investigated by means of kinetic Monte Carlo method based on transition-state theory. Using ab-initio determined exchange parameters and spin moments we apply the irreducible tensor operator technique to evaluate the Heisenberg-Dirac-Van Vleck quantum spin Hamiltonian for calculation of magnetic susceptibility of atomic chains. Using this value as a macroscopic entanglement witness we demonstrate that in antiferromagnetic chains of different length the entanglement temperature can be as much as 30-40 K.

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