

EMERGING MAGNETISM IN ULTRATHIN 4D AND 5D TRANSITION METAL NANOWIRES

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We have performed full-potential, fully relativistic, spin-polarized, all-electron density-functional calculations for monoatomic nanowires of the 4*d* and 5*d* transition metals Ru, Rh, Pd, Ag, Os, Ir, Pt and Au. Both straight and zig-zag wires were investigated, and we find that the magnetic moment as well as the number of conductance channels are highly dependent on the precise geometry of the wire, which in turn depends on the forces exerted on the wire. The spin-orbit coupling was found to be crucial for a correct description of the 5*d* wires.