Magnetic properties of Pd atomic clusters from different theoretical approaches

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Abstract

We report a comparative study of the magnetic properties of free-standing Pd_N clusters ($2 \leq N \leq 21$) obtained through two different theoretical approaches that are extensively employed in electronic structure calculations: a semi-empirical Tight-Binding (TB) model and an ab-initio DFT pseudopotential model. Conclusions are drawn about the reliability of the TB model for the investigation of the electronic structure and magnetic properties of such complex 4d Transition Metals (TM) systems and we compare the results with previous systematic DFT calculations and comment on some available experiments in the literature.