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Spin-dependent Otto quantum heat engine based on a molecular substance WOLFGANG HÜBNER, GEORGIOS LEFKIDIS, CHUANDING DONG, DEBAPRIYA CHAUDHURI, University of Kaiserslautern and Research Center OPTIMAS, LEVAN CHOTORLISHVILI, JAMAL BERAKDAR, Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany — We explore the potential of single molecules for thermodynamic cycles[1]. To this end we propose two molecular heat engines based on the realistic Ni_2 dimer: a quantum Otto engine and a modified quantum Otto engine for which laser-induced optical excitations substitute for one of the heat-exchange points. For reliable predictions and to inspect the role of spin and electronic correlations we perform fully correlated *a*b initio calculations of the electronic structure and the excited states. We analyze the efficiency and the word output of the derived engines and find an enhancement when the spin degree of freedom is included. We also use the von Neumann entropy to describe correlations and entanglement of the engines during the cycles. Furthermore, we link our results to previous results regarding an isobaric stroke[2] and a magnetic quantum Diesel engine on the same substance[3].

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