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The Otto thermodynamic cycle using the magnetic molecule Ni_2
WOLFGANG HÜBNER, CHUANDING DONG, GEORGIOS LEFKIDIS, Dept. of Physics and Research Center OPTIMAS, University of Kaiserslatern — In order to design realistic molecular heat engines, the study of quantum thermodynamics is essential since classical thermodynamics does not apply in this extreme miniaturization limit [1,2]. Realizing a thermodynamic cycle on an existing magnetic molecule embodies a novel and unique approach to understand and exploit the thermodynamic properties of spin at the molecular level.
Here we propose an Otto cycle in the Ni_2 dimer based on a fully ab-initio calculation of the electronic states and the perturbative inclusion of spin-orbit coupling. A laser pulse, described by the time-dependent Schrödinger equation, is used to heat the Ni_2 dimer. The pulse not only excites the electrons to higher, many-body electronic states, but also influences the spin of the system due to spin-orbit coupling. Using a low-temperature thermal bath the system is cooled back to the ground state. The adiabatic work exchange between the Ni_2 and the environment is described by the quasi-static expansion or compression of the bond length of the dimer. The calculated efficiency of the cycle is up to 34%.
[1] T. D. Kieu, Phys. Rev. Lett. **93** 140403 (2004)
[2] H. T. Quan, Phys. Rev. E **79** 041129 (2009)
[3] T. Zhang *et al.*, Phys. Rev. A **75** 062102 (2007)

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