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Using laser-induced spin manipulation to build magnetic nanologic elements

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Abstract. We present an \textit{ab initio} theory of ultrafast nanologic elements and show that controlled spin manipulation is feasible with the inclusion of spin-orbit coupling in $\Lambda$-processes. We show that in branched metallic chains with three magnetic centers both spin flips and spin transfers are possible within a hundred femtoseconds. A static external magnetic field and the magnetic state of one magnetic center serve as input poles (input bits), while the magnetic state of the cluster after a controlled laser pulse can be mapped to the output. Combining laser-induced spin-manipulation scenarios we are able to construct the NAND logic. Thus multicenter magnetic clusters can extend spin dynamics to optically triggered and functionalized magnetic transport on a subpicosecond timescale and nanometer spatial scale.

1. Introduction
Today computer technology advances with a such a pace that the size and speed limits of the currently used materials have almost been reached. This dictates the search for new technologies that could replace the existing electric-charge-based transistors. To this end magnetic logic seems to be an appealing alternative since, one can use one spin every about 10 atoms, instead of about one elementary electric charge every $10^4$ atoms in the existing semiconductors. This advantage can both shrink the magnetic logic elements and boost up their performance.

Ever since the ultrafast demagnetization of magnetically ordered materials was discovered \cite{1} both theoretical and experimental investigations have been intensified in the search of ultrafast spin manipulation. Most of the experiments deal either with macroscopic magnetic effects, however, such as magnetoresistive elements \cite{2}, magnetic-domain-wall logic \cite{3}, and majority logic gates for magnetic quantum dots \cite{4}, or investigate small structures where the cation concentrations are responsible for the logic operations of the microscopic structures \cite{5}. The experimental evidence of laser-driven ultrafast magnetic manipulation in (anti)ferromagnetic materials \cite{1, 6} motivates the design of a cluster with more than one magnetic center which allows for spin manipulation both spectroscopically and spatially resolved (both spin switch and spin transfer).

In the present paper we theoretically investigate the possibility of using three-magnetic-center clusters in order to build magnetic logic elements and we present a NAND gate, one of the two basic logic gates (along with NOR gate) from which any other logic gates can be built. Note also that FLASH memory realizations as well need either NAND or NOR gates.
2. Theory

The first ingredient of a magnetic logic element (in analogy to the conventional transistors) is the ability to locally store a bit of information (spin up or spin down), trigger the logical information (shine with the laser pulse) and finally read the output (again spin up or spin down). To this end one needs to be able to differentiate between input and output poles. These can consist of the same magnetic center in the cluster (but temporally separated, i.e. state before and after the logic operation) or, preferably spatially separated, that is different parts of the cluster can be interpreted as input or output parts of the logic elements. In either case spin transfer is essential as in conventional logic elements based on electronic transport. The second ingredient is the operational dynamics. From our previous works one sees that the laser pulses can indeed trigger and drive ultrafast spin dynamics. What is necessary is the presence of spin-orbit coupling (SOC, which serves as a spin-mixing mechanism), and an external magnetic field, which energetically separates ”spin-up” and ”spin-down” states (Zeeman effect [7]).

Our main idea relies on treating spin switch and spin transfer on equal footings. In order to locally switch the spin, we take advantage of a laser-induced Λ-process; i.e. we coherently excite the electronic state of our cluster from a spin-down to a spin-mixed excited state and then deexcite it to the ground state with the opposite spin. This procedure works as long as one finds energetically low lying states with a spin density localized on one single magnetic center [8, 9]. Spin transfer is possible with Λ-processes if one chooses initial and final states with different spin-density localizations rather than different spin directions. In principle one could also think of simultaneously transferring and switching the spin, however in all the cluster families investigated up to now this seems not to be possible [8, 9, 10, 11].

The theoretical calculations take place in three steps: (a) many-electron highly correlational non-relativistic calculations are performed on the structures. This is necessary in order to correctly describe the many-body nature of the wavefunctions and obtain correct energy values for the excited states. Furthermore (and more importantly) in our calculations magnetic order arises from the combination of the electronic correlations (due to the electron-electron interactions) and the Pauli exclusion principle. (b) SOC and a static external magnetic field are added in a perturbative way, and (c) dynamics is switched on by means of time-dependent perturbation theory. The difficulty lies not only in choosing the cluster and designating the appropriate states but in tailoring the laser pulse and in choosing a suitable excited state as well. The latter must be addressable from both the initial and the final state with transition matrix elements of comparable magnitudes, otherwise the Λ-process transmutes into a simple Rabi oscillation. To this end a special genetic algorithm was developed [8].

3. Results

We investigate a family of metallic clusters with three magnetic centers (Fe, Co, and/or Ni) which are interconnected with Na-chains. We set the distance between the atoms to 3.6 Å, the lattice constant of the Cu(001) surface that can be used as a fictitious ”inert” substrate. It is important that the cluster be asymmetric so that the the many-body wavefunctions, the spin density of which is localized on different centers, are nondegenerate and therefore distinguishable. Additionally, we add one branching in the chain so that the magnetic centers are always ”terminating” the chains. Last but not least is the number of the Na atoms, which, although nonmagnetic, contribute an odd number of electrons and can therefore be chosen to arrive at an even total number, if one wants to deal with singlet and triplet states (the latter, unlike doublets, facilitate spin-charge separation). The first striking non-expected result is that most magnetic states have the spin density localized at a single magnetic center. Subsequently we define the easy axes for every state as the direction of an infinitesimal external B-field for which the energy reaches its minimum. It is interesting to note that the spins mostly point in-plane, and that two out of the three magnetic centers exhibit almost collinear spins while the
Figure 1. (Color online) Left Panel: some of the clusters investigated. The arrows denote the easy axes of the spins when they are localized at the respective atoms. The numbers next to the arrows show the respective states. Note that the easy axis of the Co in NiNa$_2$(Ni)NaCo (left cluster) is perpendicular to the plane. Right Panel: level schemes of the clusters. The black solid lines are the triplet (magnetic) states, and the dashed red lines the singlet states. The arrows denote the intermediate excited states used in spin manipulations.

Table 1. Some of the lowest levels of the NiNa(Ni)Na$_2$Co chain, with a static external field along the easy axis of the ground state (in-plane at a 22.4° angle to the main Ni-Co axis). $\langle M_{tot} \rangle$ is always in-plane, the angle is given with respect to the external field.

| State | Energy (eV) | $\langle M_{tot} \rangle$ | Angle | Spin localization |
|-------|-------------|--------------------------|------|-------------------|
| 14    | 0.8729      | 2.873                    | -23.7| Co                |
| 13    | 0.8710      | 2.873                    | 156.5| Co                |
| 8     | 0.1501      | 2.000                    | 68.1 | middle Ni         |
| 7     | 0.1497      | 2.000                    | -111.8| middle Ni        |
| 6     | 0.0773      | 2.745                    | 68.3 | middle Ni         |
| 5     | 0.0764      | 2.745                    | -112.0| middle Ni        |
| 4     | 0.0747      | 0.987                    | 0.1  | edge Ni           |
| 3     | 0.0725      | 0.987                    | -179.9| edge Ni         |
| 2     | 0.0022      | 2.879                    | 0.2  | edge Ni           |
| 1     | 0.0000      | 2.879                    | -179.8| edge Ni         |

spin of the third one points in an perpendicular usually coplanar direction (Fig. 1). Typically we find that the lowest lying many-body states originate from triplets (after inclusion of SOC- and Zeeman-splitting). Thus below 1 eV we always find at least one "spin-up" and one "spin-down" state for every magnetic center, plus several non-magnetic ones. Note that "spin-up" or "spin-down" merely means that, although $S$ is not a good quantum number, the expectation value of its projection along the respective easy axis $\hat{q}$ is in the vicinity of ±1.8.

There are some unique findings in the NiNa$_2$Ni$_2$ cluster: (a) There exists a static magnetic field orientation which allows for a spin transfer from the middle Ni atom to the edge Ni atoms, but not for a spin flip. This fact can be used for controlling the localization of the spin in the process of the intended logical operations without loss of the overall spin orientation. (b) The local spin flip at the edge Ni atom is approximately 5 times slower (ca 450 fs) than at the middle atom (ca 100 fs). This difference can be used to selectively flip the spin depending on the localization of the spin by simply using a pulse which is large enough to flip the spin only if it is located at the middle atom but not at the edge Ni (note that only one of the edges
Table 2. NAND gate. We put in the spin at the edge Ni and the orientation B field and read the middle Ni "down" state. We exploit the fact that transfer is only possible if the magnetic field is parallel to the long molecular axis.

| input 1 (spin) | input 2 (B-field) | output (spin+position) |
|----------------|-------------------|------------------------|
| 1 (edge↑)     | 1 (parallel)      | 0 (middle↑)            |
| 0 (edge↓)     | 1 (parallel)      | 1 (middle↓)            |
| 1 (edge↑)     | 0 (tilted)        | 1 (edge↑)              |
| 0 (edge↓)     | 0 (tilted)        | 1 (edge↓)              |

is interesting since the other one is "isolated" in the sense that no spin transfer from and to it is possible). The NiNa$_2$(Ni)NaCo cluster behaves similarly. In the former one, however, the resonances needed for the transfer and flip processes differ sufficiently to make them controllable through explicit access of the intermediate excited states while in the latter one both processes go through the same state (see the arrows in Fig. 1). In the case of the cluster with two Co atoms a controlled flip or transfer is generally not possible because the states suited for the different processes are bunched together (around 3 eV) and interfere destructively. Thus we could not explicitly address a suitable state without simultaneously initiating other undesired processes. NiNa$_2$Ni$_2$ is the only cluster up to now, for which both spin transfer and spin switch have been achieved. Furthermore, the processes in question are possible only with very specific combinations of the external B-field and the laser propagation, thus allowing for logic operations. We use the magnetic state of the lower Ni and the orientation of the static magnetic field as the input bits and we read the magnetic state of the middle Ni as an output bit. Thus we can map ultrafast spin-manipulation scenarios to a NAND gate (Tab. 2). We have also been able to construct an OR, an XOR and two AND gates from the same cluster (see Ref. [11]).

4. Conclusions
We have shown that with the use of an external magnetic field and properly tailored laser pulses, it is possible to construct ultrafast magnetic nanologic elements by exploiting laser-induced Λ-processes and SOC and by using the spin density of one center and the orientation of the static magnetic field as input bits and the spin density on a different center as the output bit. This way we presented a prototypic magnetic-logic NAND gate based on a sufficiently realistic material which can be used for constructing magnetic-based quantum computer circuits.

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