Quantum Spintronics : Study of electron correlation in linear doped Nickel oxide chains - An exact diagonalization and DMRG study

Matilde POUYOT*,†,‡ and Vijay Gopal CHILKURI*,†

†*Department of Chemistry, Aix-Marseille University,*

‡*A shared note*

E-mail: matilde.pouyot@etu.univ-amu.fr; vijay-gopal.chilkuri@univ-amu.fr

Phone: +123 (0)123 4445556. Fax: +123 (0)123 4445557

Abstract

This is an example document for the *achemso* documentclass, intended for submissions to the American Chemical Society for publication. The class is based on the standard LaTeXe *report* file, and does not seek to reproduce the appearanceof a published paper. This is an abstract for the *achemso* document class demonstration document. An abstract is only allowed for certain manuscript types. The selection of `journal` and `manuscript` will determine if an abstract is valid. If not, the class will issue an appropriate error.This is the abstract.

Introduction

The Nickel-Oxide compound is a linear compound and has the following electronic structure shown in Figure 1. The two valence orbitals i.e. d_{z^2} and $d_{x^2-y^2}$ are singly occupied and quasi degenerate[1].

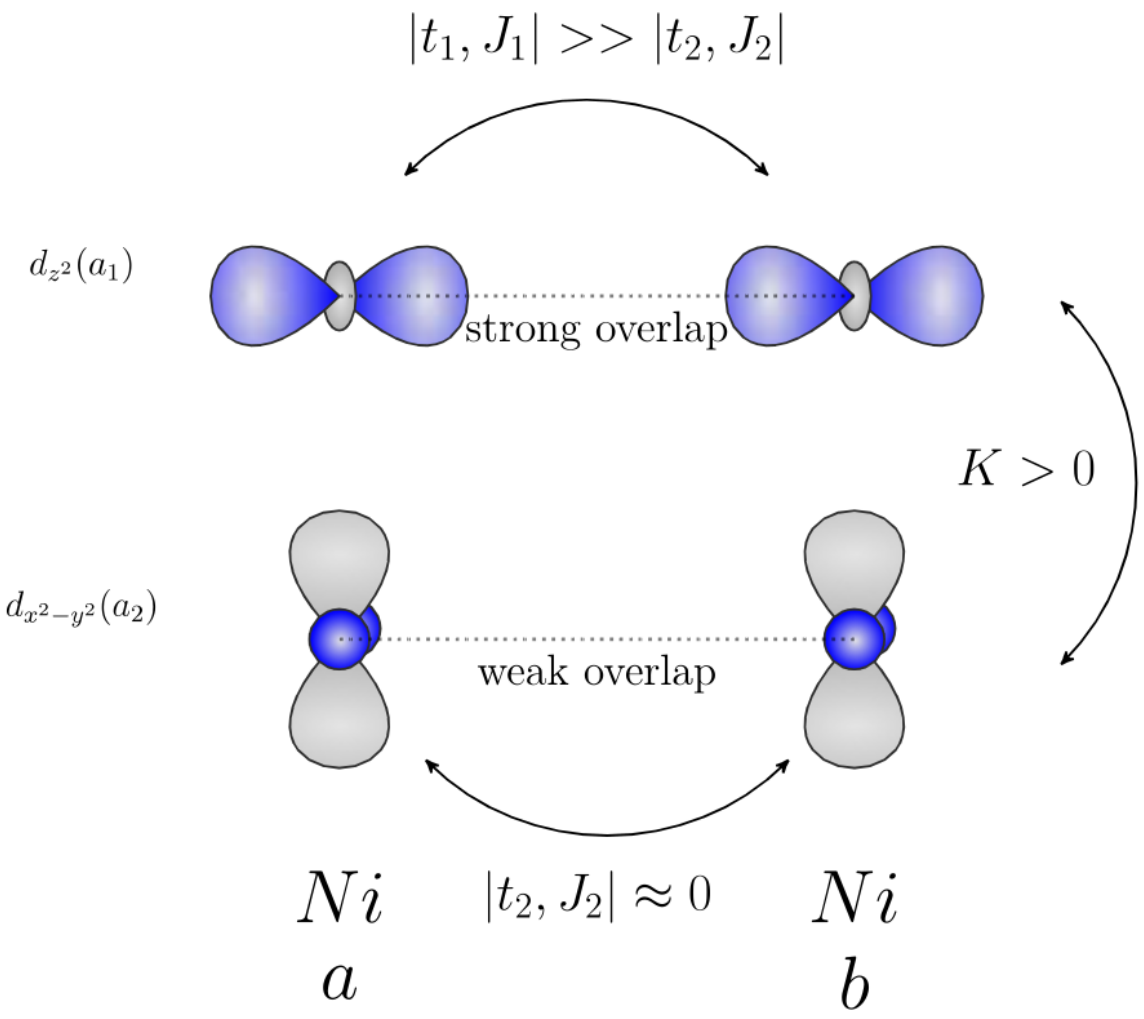

Figure 1: Valence electronic structure of Ni(II) ion in the $[Ni_2(napy)_4Br_2]$ compound.

These orbitals imply the existance of two types of electrons. The first, occupying the d_{z^2} orbitals, are delocalized along the linear axis (i.e. the z axis). Second, those occupying the $d_{x^2-y^2}$ orbitals, are localized on the nickel atoms. These two types of electrons therefore, render this compund a suitable candidate for spintronics applications.

The model frequently used to describe such molecules is known as the Double Exchange model (DE)[2] as shown in Equation 1.

$$\hat{H}_{DE} = -\sum_{i} 2K \left(\hat{S}_{ai} \cdot \hat{S}_{bi} - \frac{\mathbb{1}}{4}\right) \delta_{ni,2} - \sum_{\langle ij \rangle} 2J \left(\hat{S}_{ai} \cdot \hat{S}_{aj} - \frac{\mathbb{1}}{4}\right) \delta_{ni,nj} + \sum_{\langle ij \rangle} t \left(\hat{a}^{\dagger}_{ai} \cdot \hat{a}_{aj} \delta_{ni(ni+1)} + h.c.\right) \tag{1}$$

Sophisticated models also include the long-range repulsion between the electrons as done also for example in the Pariser-Parr-Pople (PPP) hamiltonians called V_{ij}. This is a diagonal operator and is written as shown in Equation 2.

$$\hat{H}_{PPP} = \hat{H}_{DE} + \sum_{\langle ij \rangle} V_{ij} \hat{n}_i \cdot \hat{n}_j \tag{2}$$

Along with these two models, one can simulate collective properties of the linear chain nickel-oxide compounds.

These interactions are shown schematically in Figure 2, where each site represents one nickel atom. Since the compound can be doped with positive charges, each nickel atom can have either two or one electron as shown in Figure 2. The 30 states of this model can be subdivided into two family of states:

1. Family 1, where the hole (i.e. the empty orbital) resides in an orbital of type 1 (i.e. the a_1 or d_{z^2} orbital).
2. Family 2, where the hole resides in an orbital of type 2.

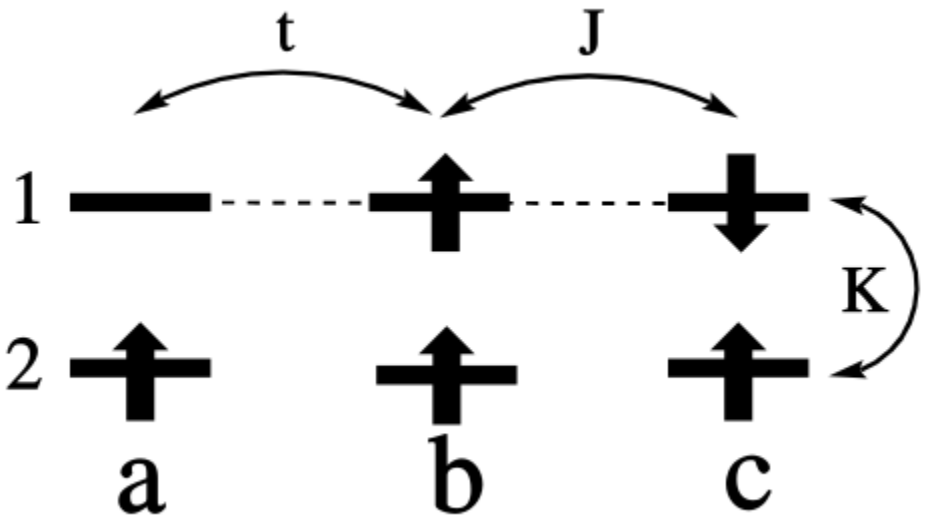

Figure 2: A schematic of the different interactions in the double-exchange model hamiltonian.

The two family of states do not interact with each other due to symmetry. In the DE model, we shall study the states belonging to Family 1 only because the ground state and few low lying excited states belong to this family as shown in Figure 3.

In the present work, we shall investigate the collective properties of linear chanins of variable lengths and doping ratios.

As an example, for the case of three sites (Figure 2), one can write down the double-exchange matrix Equation 1 for the three sextet states as shown in Table 1.

Table 1: The matrix for the sextet spin-block.

$\hat{H}_{sext}$	$\|S_1\rangle$	$\|S_2\rangle$	$\|S_3\rangle$
$\langle S_1\|$	0	$-t$	0
$\langle S_2\|$	$-t$	0	$-t$
$\langle S_3\|$	0	$-t$	0

Similarly, for the quartet states, the matrix is given in Table 2.

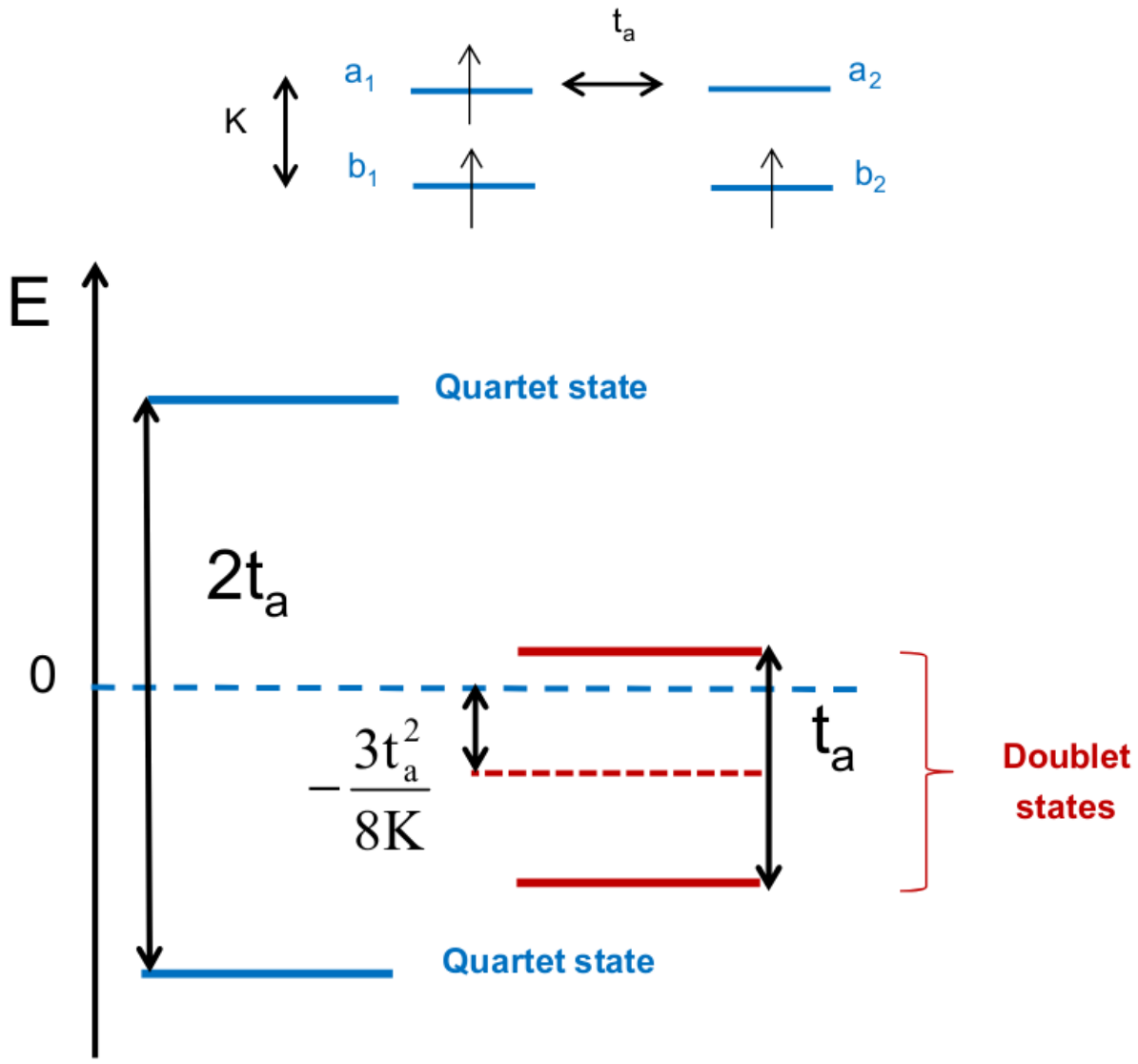

Figure 3: Comparison of the relative energies of the states belonging to Family 1 and Family 2.

Table 2: The matrix for the ms 0 spin-block.

-j	0	0	0	j	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	2 k-j	-k	-k	0	j	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	-k	2 k	0	-k	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	-k	0	2 k	-k	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
j	0	-k	-k	2 k-j	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	j	0	0	0	-j	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	k-j	-k	0	j	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	-k	k	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	k	-k	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	0	0	j	0	-k	k-j	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	0
-t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0
0	-t	0	0	0	0	0	0	0	0	0	k	-k	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0
0	0	-t	0	0	0	0	0	0	0	0	-k	k	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0
0	0	0	-t	0	0	0	0	0	0	0	0	0	2 k	-k	0	-k	0	0	0	0	0	0	0	-t	0	0	0	0	0
0	0	0	0	-t	0	0	0	0	0	0	0	0	-k	2 k	0	0	-k	0	0	0	0	0	-t	0	0	0	0	0	0
0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	k	0	0	-k	0	0	0	0	0	0	-t	0	0	0	0
0	0	0	0	0	0	-t	0	0	0	0	0	0	-k	0	0	2 k	-k	0	0	0	0	0	0	0	0	-t	0	0	0
0	0	0	0	0	0	0	-t	0	0	0	0	0	0	-k	0	-k	2 k	0	0	0	0	0	0	0	0	-t	0	0	0
0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	-k	0	0	k	0	0	0	0	0	0	0	0	0	-t	0
0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-t
0	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	k-j	-k	0	j	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	-k	k	0	0	0	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	-j	0	0	j	0	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	j	0	0	k-j	0	0	-k	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	0	0	0	2 k	-k	0	-k	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	j	0	-k	2 k-j	0	0	-k	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	-k	0	0	k	0	0	0	0
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	-k	0	0	2 k-j	-k	j	
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	-k	0	-k	2 k	0	
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-t	0	0	0	0	0	0	0	j	0	-j	

Physical meaning of model parameters

The coulomb parameter J represents the inter-site anti-ferromagnetic coupling between the electrons occupying the d_{z^2} orbital on each site (a_1, a_2). This interaction shown schematically in table Table 3 for two sites.

Table 3: The J block of the matrix for two electrons in two sites.

$\hat{H}_J$	$\lvert a_1\bar{a}_2\rangle$	$\lvert\bar{a}_1 a_2\rangle$
$\langle a_1\bar{a}_2\rvert$	J	$-J$
$\langle\bar{a}_1 a_2\rvert$	$-J$	J

Therefore, a negative value of J stabilizes the singlet state by $2J$ compared to the triplet state.

Table 4: The eigenvalues and eigenvectors of the matrix for J.

E	$\lvert a_1\bar{a}_2\rangle$	$\lvert\bar{a}_1 a_2\rangle$
$(S=1)0$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$
$(S=0)2J$	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$

Similarly, the exchange term K exists between the two orbitals on the *same* site (a, b) as shown in Table 5. This results in the separation of the *local* singlet and triplet configurations on each site. The K interaction stabilises the triplet configuration by $2K$ compared to the local singlet configuration (Table 6).

Table 5: The K block of the matrix for two electrons on the *same* site.

$\hat{H}_K$	$\lvert a\bar{b}\rangle$	$\lvert\bar{a}b\rangle$
$\langle a\bar{b}\rvert$	K	$-K$
$\langle\bar{a}b\rvert$	$-K$	K

Table 6: The eigenvalues and eigenvectors of the matrix for K.

E	$\|a\bar{b}\rangle$	$\|\bar{a}b\rangle$
$(S=0)2K$	$\frac{1}{\sqrt{2}}$	$-\frac{1}{\sqrt{2}}$
$(S=1)0$	$\frac{1}{\sqrt{2}}$	$\frac{1}{\sqrt{2}}$

Results and discussion

Outline

The document layout should follow the style of the journal concerned. Where appropriate, sections and subsections should be added in the normal way. If the class options are set correctly, warnings will be given if these should not be present.

References

The class makes various changes to the way that references are handled. The class loads `natbib`, and also the appropriate bibliography style. References can be made using the normal method; the citation should be placed before any punctuation, as the class will move it if using a superscript citation style[3]. The use of `natbib` allows the use of the various citation commands of that package have shown something. Long lists of authors will be automatically truncated in most article formats, but not in supplementary information or reviews. If you encounter problems with the citation macros, please check that your copy of `natbib` is up to date. The demonstration database file `bibliography.bib` shows how to complete entries correctly.

Multiple citations to be combined into a list can be given as a single citation. This uses the `mciteplus` package. Citations other than the first of the list should be indicated with a star.

The class also handles notes to be added to the bibliography. These should be given in place in the document. As with citations, the text should be placed before punctuation. A note is also generated if a citation has an optional note. This assumes that the whole work has

already been cited: odd numbering will result if this is not the case .

Floats

New float types are automatically set up by the class file. The means graphics are included as follows (Figure 4). As illustrated, the float is `here` if possible.

Your scheme graphic would go here: `.eps` format for LaTeX, or `.pdf` (or `.png`) for pdf\LaTeX < smallcaps chemdraw > files are best saved as `.eps` files: these can be scaled without loss of quality, and can be converted to `.pdf` files easily using `eps2pdf`.

Figure 4: An example scheme

As well as the standard float types `table` and `figure`, the class also recognises `scheme`, `chart` and `graph`.

Figure 5: A second example figure

Charts, figures and schemes do not necessarily have to be labelled or captioned. However, tables should always have a title. It is possible to include a number and label for a graphic without any title, using an empty argument to the `\caption` macro.

The use of the different floating environments is not required, but it is intended to make

document preparation easier for authors. In general, you should place your graphics where they make logical sense; the production process will move them if needed.

Math(s)

The `achemso` class does not load any particular additional support for mathematics. If packages such as `amsmath` are required, they should be loaded in the preamble. However, the basic LaTeX math(s) input should work correctly without this. Some inline material $y = mx + c$ or $1 + 1 = 2$ followed by some display.

$$A = \pi r^2$$

It is possible to label equations in the usual way (Equation 3).

$$\frac{\mathrm{d}}{\mathrm{d}x} r^2 = 2r \tag{3}$$

This can also be used to have equations containing graphical content. To align the equation number with the middle of the graphic, rather than the bottom, a minipage may be used.

$$\begin{array}{c}\text{As illustrated here, the width of}\\ \text{the minipage needs to allow some}\\ \text{space for the number to fit in to.}\end{array}$$

Experimental

The usual experimental details should appear here. This could include a table, which can be referenced as Table 7. Notice that the caption is positioned at the top of the table.

Table 7: An example table

Header one	Header two
Entry one	Entry two
Entry three	Entry four
Entry five	Entry six
Entry seven	Entry eight

You may add footnotes to ables as illustrated (Table 8).

Table 8: An example table with notes

Header one	Header two
Entry one[1]	Entry two
Entry three[2]	Entry four
Entry five	Entry six
Entry seven	Entry eight

The example file also loads the optional `mhchem` package, so that formulas are easy to input: `[H2SO4]{.ce}` gives H_2SO_4. See the use in the bibliography file (when using titles in the references section).

The use of new commands should be limited to simple things which will not interfere with the production process. For example, `\textbackslash mycommand` has been defined in this example, to give italic, mono-spaced text: ***some text***.

[1]This is a footnote

[2]This is a second note

Extra information when writing JACS Communications

When producing communications for *J.~Am. Chem. Soc.*, the class will automatically lay the text out in the style of the journal. This gives a guide to the length of text that can be accommodated in such a publication. There are some points to bear in mind when preparing a JACS Communication in this way. The layout produced here is a *model* for the published result, and the outcome should be taken as a *guide* to the final length. The spacing and sizing of graphical content is an area where there is some flexibility in the process. You should not worry about the space before and after graphics, which is set to give a guide to the published size. This is very dependant on the final published layout.

You should be able to use the same source to produce a JACS Communication and a normal article. For example, this demonstration file will work with both `type=article` and `type=communication`. Sections and any abstract are automatically ignored, although you will get warnings to this effect.

Acknowledgement

Please use "The authors thank …" rather than "The authors would like to thank …".

The author thanks Mats Dahlgren for version one of `achemso`, and Donald Arseneau for the code taken from `cite` to move citations after punctuation. Many users have provided feedback on the class, which is reflected in all of the different demonstrations shown in this document.

Supporting Information Available

This will usually read something like: "Experimental procedures and characterization data for all new compounds. The class will automatically add a sentence pointing to the information on-line:

References

(1) Guihéry, N.; Malrieu, J. P. The double exchange mechanism revisited: An ab initio study of the [Ni2(napy)4Br2]+ complex. *The Journal of Chemical Physics* **2003**, *119*, 8956–8965.

(2) Chilkuri, V. G.; Suaud, N.; Guihery, N. High-Spin Chains and Crowns from Double-Exchange Mechanism. *Crystals* **2016**, *6*, 1–15.

(3) Garnier, S.; Gautrais, J.; Theraulaz, G. The biological principles of swarm intelligence. *Swarm Intelligence* **2007**, *1*, 3–31.