Magnetic properties of deposited Polyoxometalates

Jürgen Schnack

Department of Physics - University of Osnabrück

http://obelix.physik.uni-osnabrueck.de/∼schnack/

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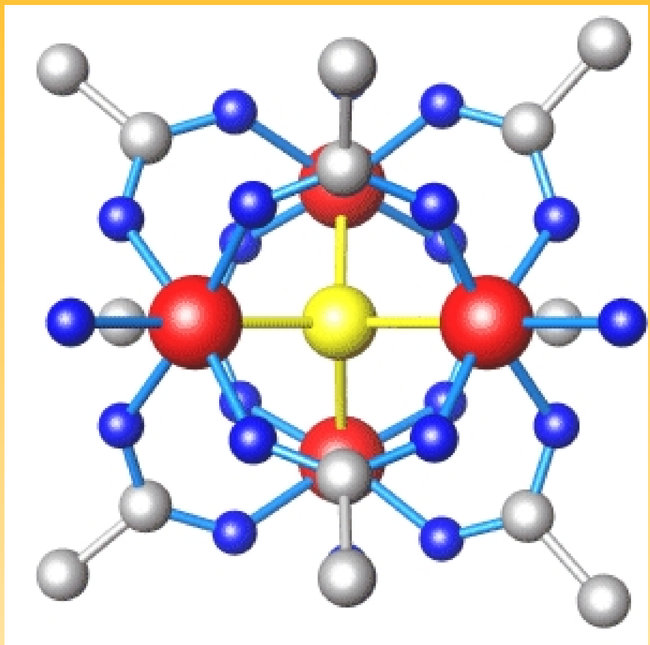
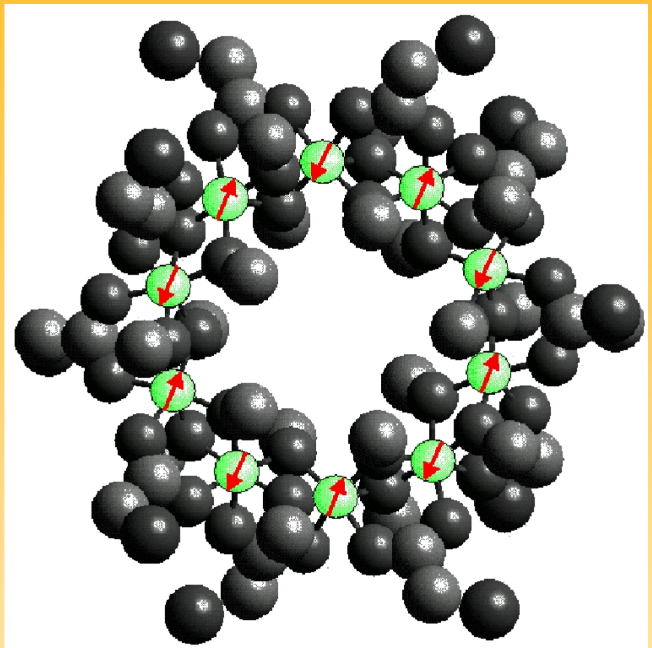
Contents

What are magnetic molecules?



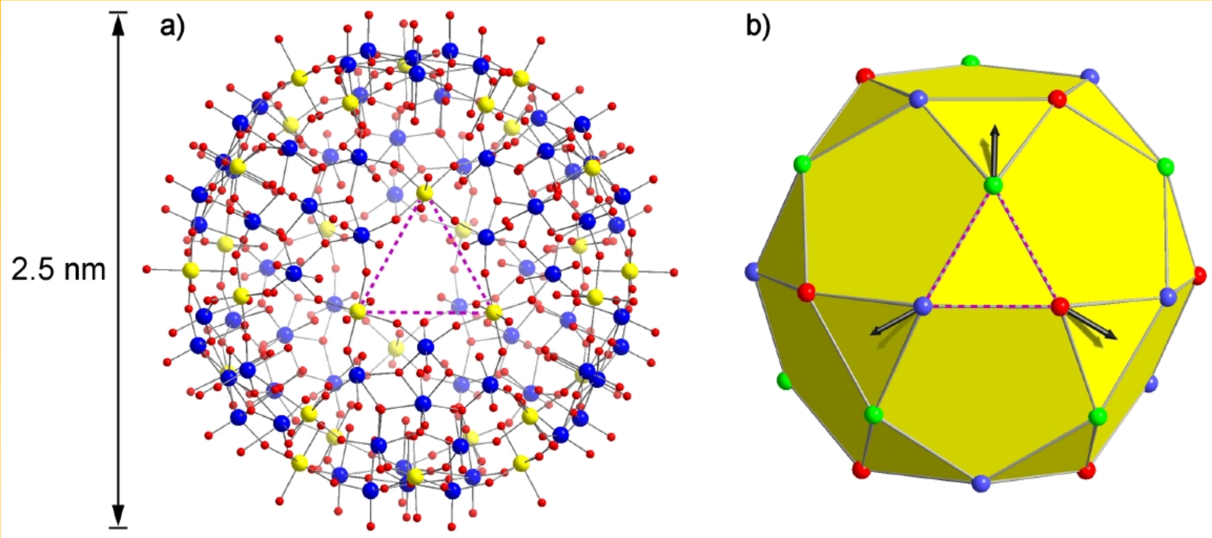
- macro molecules, e.g. polyoxometalates: consist of constituents like Hydrogen (H), Carbon (C) and Oxygen (O) as well as paramagnetic ions like Iron (Fe), Chromium (Cr), Copper (Cu), Nickel (Ni) or Manganese (Mn);
- pure organic magnetic molecules: magnetic coupling between high spin molecules (e.g. free radicals);
- intermolecular interaction relatively small.

Structure of magnetic molecules



- dimers (Fe_2), tetrahedra (Cr_4), cubes (Cr_8);
- rings, especially iron rings (Fe_6, Fe_8, Fe_{10}, ...);
- complex structures (Mn_{12});
- soccer balls, more precisely icosidodecahedra (Fe_{30}) and other macro molecules.

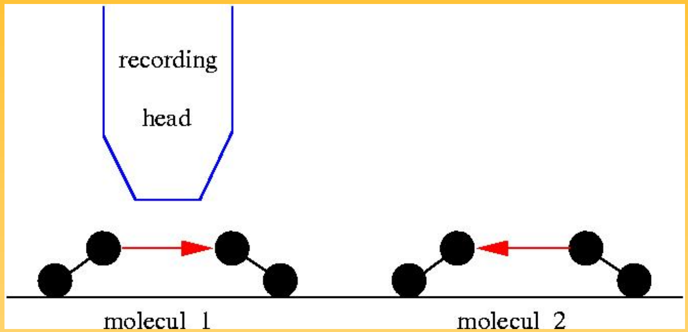
Example for magnetic macro molecules $\{Mo_{72}Fe_{30}\}$

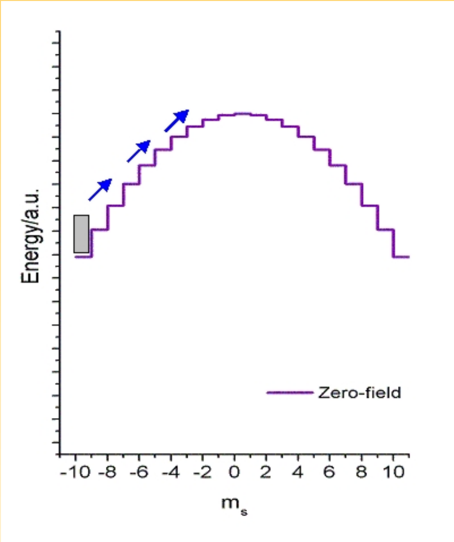


- structure of $\{Mo_{72}Fe_{30}\}$: Fe - yellow, Mo - blue, O - red,
- antiferromagnetic interaction mediated by O-Mo-O bridges.

- classical ground state of $\{Mo_{72}Fe_{30}\}$: three sublattice structure, coplanar spins,
- quantum mechanical ground state $S = 0$ can only be approximated, dimension of Hilbert space $(2s+1)^N \approx 10^{23}$.

Magnetic molecules as storage media?

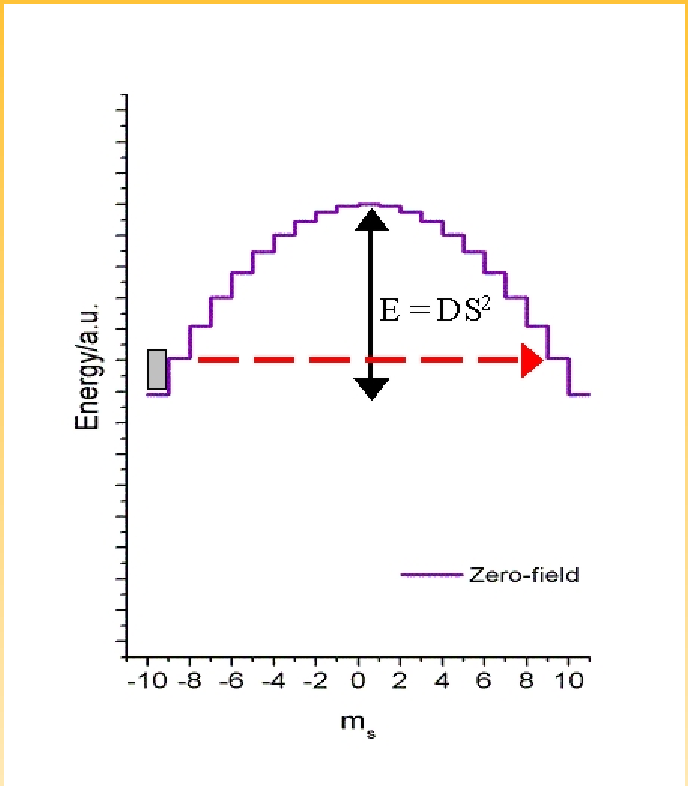




Advantages:

- every molecule is a domain of its own; very weak intermolecular interactions; high density and nevertheless good separation of magnetic moments;
- high spin possible, e.g. $S = 10$;
- magnetic molecules show hysteresis;
- theoretically possible storage density:
  40 Tbits per square inch,
  today: 20 Gbits per square inch (IBM), 300GB per square inch (Fujitsu 05/2002)

Magnetic molecules as storage media?

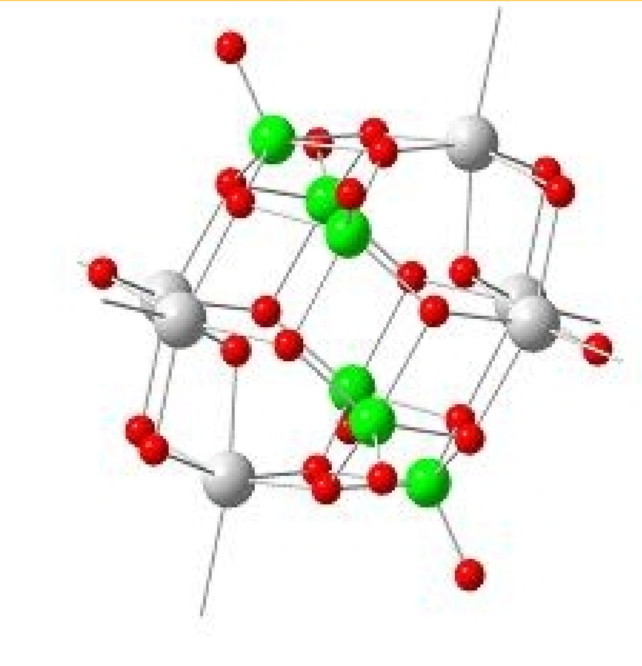


Disadvantages:

- magnetisation tunneling! stabilisation by appropriate substrate?
(Prof. Blügel, Osnabrück/Jülich, http://www.flapw.de)
- often very small coupling ($J \approx 10$ K), i.e. thermally unstable at room temperature;
- recording head must be very small and needs precise guide.

http://www.people.man.ac.uk/~mbdssrew/winpeny_intro3.html

Aims of the project



- effective spin Hamiltonian for the molecule synthesized by H. Reuter/M. Izaaryene;
- possible application of magnetic molecules: storage devices; therefore dynamics of the magnetization due to thermal activation, disturbance by phonons, and under the influence of an external magnetic field are of utmost importance;
- magnetic molecules in time-dependent magnetic fields;
- influence of phonons on the interaction Hamiltonian of magnetic molecules.

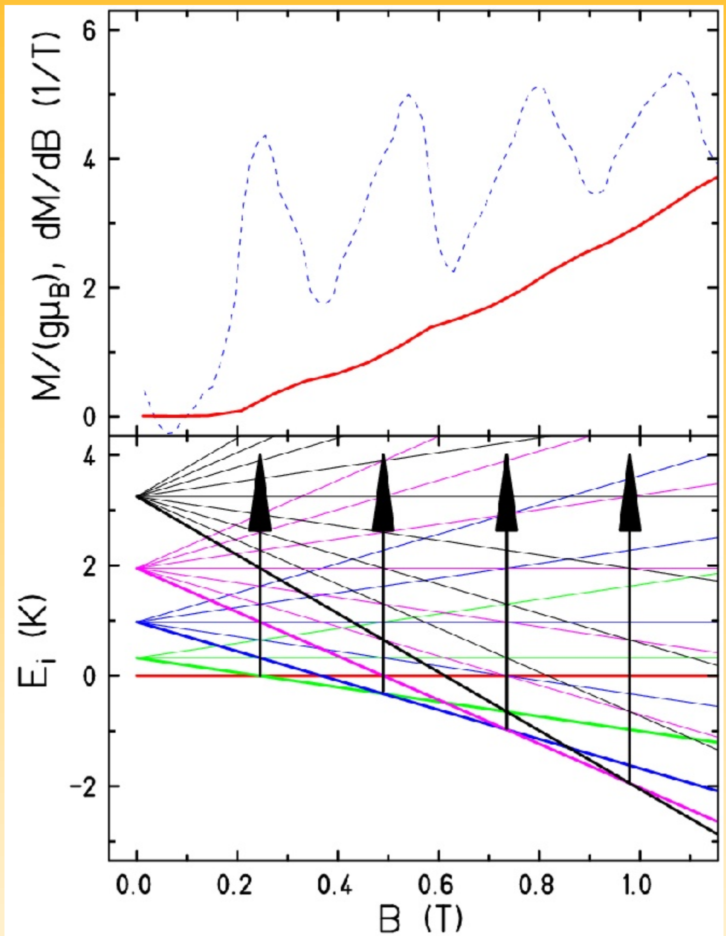
Model Hamiltonian – Heisenberg-Model

$$\underset{\sim}{H} = -\sum_{i,j} J_{ij}\,\underset{\sim}{\vec{s}}(i)\cdot\underset{\sim}{\vec{s}}(j) - D\sum_{i}\left(\vec{e}(i)\cdot\underset{\sim}{\vec{s}}(i)\right)^2 + g\,\mu_B\,B\sum_{i}^{N}\underset{\sim}{s}_z(i)$$

The Heisenberg modell including anisotropy, and dipol-dipol if necessary, as well as Zeeman term describes the magnetic spectrum of many molecules with high accuracy.

Since the dimension of Hilbert space grows with $(2s+1)^N$ the Hamiltonian can be diagonalized completely for small molecules. For larger ones approximate methods are used.

Time-dependent magnetic fields



- magnetization tunneling at avoided level crossings – description via time-dependent Schrödinger equation or Landau-Zener formula;
- ⇒ hysteresis effects;
- relaxation processes due to phonons – description with detailed balance;
- ⇒ flattens hysteresis.

Phonons and the interaction Hamiltonian

$$\underset{\sim}{H} = -\sum_{i,j} J(\vec{r}_i, \vec{r}_j)\ \underset{\sim}{\vec{s}}(i) \cdot \underset{\sim}{\vec{s}}(j)$$

$$J(\vec{r}_i, \vec{r}_j) \approx J(|\vec{r}_i - \vec{r}_j|) \approx J^{(0)}(ij) + \frac{1}{2}\delta\vec{r}_{ij} \cdot \frac{\partial}{\partial \vec{r}_{ij}} \otimes \frac{\partial}{\partial \vec{r}_{ij}} J(|\vec{r}_{ij}|) \cdot \delta\vec{r}_{ij}$$

- expected that the vibrational degrees of freedom, the phonons, do have an appreciable effect on the magnetic properties of molecular magnets, since molecular magnets can be rather soft;
- dependence of $J(|\vec{r}_{ij}|)$ on $\vec{r}_{ij}$ by SDFT + frozen phonon calculations (Prof. Blügel);
- possible magnetoelastic spin-Peierls phase transitions;
- Because of the complexity of the phonon-magnon interaction not even simple model studies have been reported so far for molecular magnets.

Thank you very much for your attention.

Collaboration

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- Prof. S. Blügel (FZ Jülich);
- Prof. J. Richter (Uni Magdeburg);
- Dr. A. Honecker (Uni Braunschweig).