FIRST PRINCIPLES ELECTRONIC STRUCTURE CALCULATIONS for NANOMATERIALS MODELING

a)National Institute for Materials Physics, Bucharest-Magurele, PO-BOX MG-07, Romania

b)National Institute for R&D in Microtechnologies-IMT Bucharest, PO-BOX 38-160, Romania

N. Plugaru[a)], R. Plugaru[b)]

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1. MOTIVATION

During the last decade, new and strong demands are posed to materials since the development of promising technologies in key domains - such as **Energy, Environment and Information Technology** - is restricted by the lack of materials with adequate properties.

Computational Materials Modeling emerges as a powerful tool in the development of future technologies.

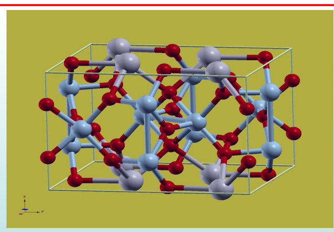
2. Density Functional Theory (DFT) Framework

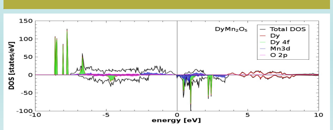
Main goal: given the chemical composition and the geometrical structure of a system, to calculate its properties by solving the electronic Schrodinger equations - a correlated many body problem (solved only approximately, yet).

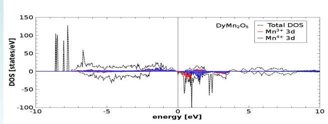
- No usage of empirical information or free parameters.

3.1 RMn2O5

- Multiferroic properties, Outstanding coupling between the magnetic and ferroelectric modes [1,2].
- Crystal structure: Infinite chains of $Mn^{4+}O6$ octahedra, linked through $[Mn^{3+}O5]$ pyramidal units and bicapped antiprisms [RO8] [3].
- Magnetic structure : Complex AF order at low T, amplitude modulated.







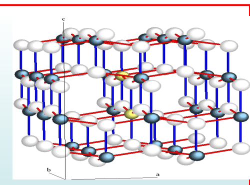
References

[1] W. Eerenstein et al., Nature 442 (2006) 759.

[2] Y Noda *et al J. Phys.: Condens. Matter* 20 (2008) 434206

[3] J.A. Alonso et al., *J. Phys.: Condens. Matter* 9 (1997) 8515.

3.2 TM:$TiO_{2-\delta}$ anatase phase.



- DMS films for spintronic devices [1].
- Evaluation of direct TM-TM exchange; OV-s role ? [2]

L(S)DA results :

- AF ground state: Mn and Fe doping;
- FM or AF for Co doping (OV-s conc.).
- TM electronic configuration: M^{2+} ;

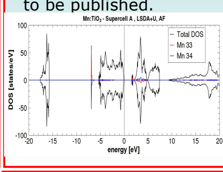
Two spin configurations of the TM may coexist

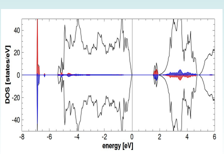
- OV-s increase by 20-30 %the direct TM-TM exchange strength.

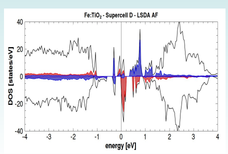
References

[1] R. Janisch, N. A. Spaldin, Phys. Rev. B 73 (2006) 035201.

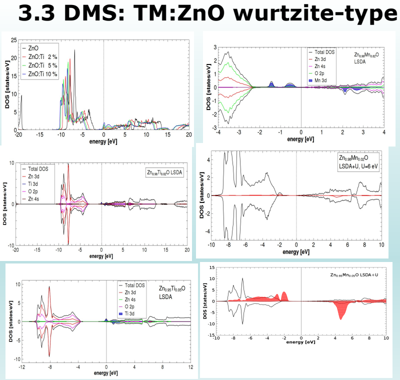
[2] N. Plugaru, R. Plugaru, Psi-k 2010 Conf., Berlin, Germany, to be published.







3.3 DMS: TM:ZnO wurtzite-type



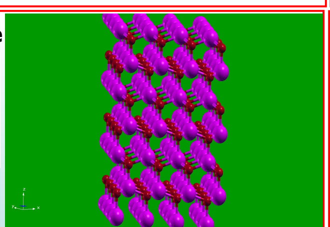


Table 1. Magnetic moment per 3d ion, m, and per formula unit, M, in Ti/Mn :ZnO.

x (3d)	(at.%)	2	5	10
m (μ_B/at)	Ti	0.90	1.13	1.28
	Mn*)	4.71 (4.97)	4.71 (4.97)	4.71 (4.97)
M (μ_B/f.u.)	Ti	0.02	0.06	0.13
	Mn	0.10	0.25	0.50

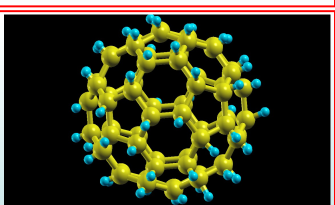
*) between paranthesis, the values from LSDA+U calculations.

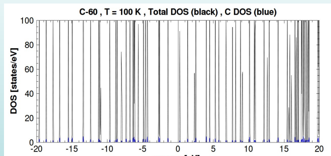
The description of electrical conductivity in disordered ZnO : a lasting challenge due to the entanglement of magnetism and charge/spin transport.

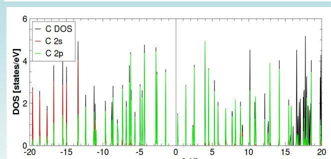
References

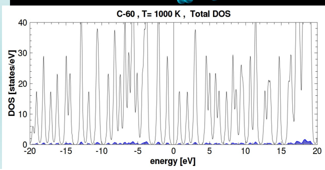
R. Plugaru and N. Plugaru, Psi-k 2010 Conf. Berlin, Germany, September 12-16, 2010. to be published.

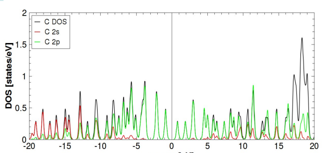
3.4 Carbon nanostructures: C60











Effect of temperature on DOS.

OUTLOOK

Three good reasons for performing Computational Materials Modeling

1. **High throughput calculations become economically relevant.**
2. **Increasing accuracy in the predictions, approaching more and more to real world.**
3. **It provides an insight where experiment has little access, if at all (materials for nuclear activities, strong fields, high pressures and temperatures, complex molecular devices, etc.)**

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