Dr Magnin Yann : Curriculum Vitae

Nationality: French
Birth: May, 1980
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Actually: Researcher Scientist MSE^2 (Multiscale Material Science for Energy & Environment)
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Scientific topics and main results

My research is focused on the modelization of graphitic, dense or porous carbonaceous structures in interaction with metallic nanoparticles. The modeling of such properties is important in different fields:

- The study of the growth mechanisms of carbon allotropes such as graphene or carbon nanotubes.

- The characterization of the diffusion and coalescence mechanisms of nanoparticles supported on carbon substrates (a important limiting factor in catalysis).

- The structural modification of nanoparticles by carbon solubilization.

- Controlling the wetting and adhesion properties of a nanoparticle on a carbon substrate via the degree of carburation of a nanoparticle.

These studies are based on numerical simulations (Monte Carlo, molecular dynamics) from the use of empirical or from a tight binding potentials developed at the fourth moment. The originality of this work compared to other "idealized" approaches where environmental effects are often neglected - lies in the development of a metal-carbon atomistic potential capable to model realistic systems allowing direct comparisons with experimental studies. Experimentally, nanoparticles are often carburized during synthesis and are usually supported on an amorphous carbon substrate, widely used in electron microscopy (TEM). These points are limiting factors for direct comparisons between experiments and theory. Indeed, solubilized carbon atoms modify the structure of the particles, their diffusion coefficients and wetting properties can even induce confinement of particles into small pores of the substrate.

Thanks to this approach, which consists in simulating a system taking into account environmental effects (a carbon support, carbon solubility in the catalyst, etc.), we have highlighted through the calculation of phase diagrams at nanoscale the existence of a new nano-phase that is typical of small nanoparticles. This result have been published in Physical Review Letter. Identification of changes in the state of matter depending on the thermodynamic and the size of nanoparticles allowed us to understand general properties and behaviors of nanoparticle/substrate interaction. These properties have allowed us to guide experimental studies of nanotube synthesis in order to control the structural properties such as tube diameter and tube length. Finally, we shed new light on chiral selectivity of carbon nanotubes, which led these results to be published in Science.

Education and scientific career

Since 2019 : Researcher Scientist, MSE^2, (Multiscale Material Science for Energy & Environment), MIT, USA.

2017 – 2019 : Postdoctorat MSE^2, MIT, USA.
Atomistic simulations of metallic nanoparticles confined in porous carbon as CMK.
Adsorption and transport simulations of n-alkanes in porous carbon structures.
Atomistic reconstruction of realistic kerogen structures from experimental data.
Collaborators : R.J-M Pellenq, F.-J Ulm

2014 – 2016 : Postdoctorat at CINaM (Centre Interdisciplinaire de Nanoscience de Marseille- CNRS UMR 7325) AMU, Campus de Luminy, Marseille, France.
Nucleation and growth mechanisms of single wall carbon nanotubes by Monte Carlo simulations.
Collaborators : C. Bichara, H. Amara, F. Ducastelle, A. Loiseau

2013 – 2014 : Postdoctorat at ILM (Institut Lumière Matière - CNRS UMR 5306) Université Claude Bernard, Lyon 1, France.
Modelization of metallic nanoparticles supported on a graphene layer epitaxied on a metallic slab by Monte Carlo simulations.
Collaborators : F. Calvo, F. Rabilloud, G.D. Förster

2011 – 2012 : Postdoctorat at APCTP (Asia Pacific Center for Theoretical Physics), POSTECH, Pohang, South Korea.
Study of long range interactions accounting large dielectrical contrasts in the distribution of counterions on highly charged biomolecule surfaces by finit elements.
Collaborators : Y.S. Jho, A. Constantinescu

2008 – 2011 : PhD at LPTM (Laboratoire de Physique Théorique et Modélisation - CNRS UMR 8089), Université de Cergy-Pontoise, France.
Defense november 3 2011 at Université de Cergy-Pontoise.
Advisor : Pr. Hung The Diep.
Spin transport in thin layers magnetic semiconductor by Monte Carlo simulations.
Teaching : 200 hours at Université de Cergy-Pontoise.

2007 – 2008 Engineer at LPP (Laboratoire de Physique des Plasmas – CNRS UMR 7648), Polytechnique, Palaiseau, France.

2006 – 2007 Master 2 of Micro et Nanotechnologies at Université Paris Sud XI, Orsay.

Responsibilities

1. PhD advisor at APCTP (Asia Pacific Center for Theoretical Physics), POSTECH, Pohang, South Korea : Yong Seok Lee.

Internship advisor at MSE^2 (Multiscale Material Science for Energy and Environment), MIT, Cambridge, USA : Hugo Nael

2. Administrator of the cluster computers at APCTP, POSTECH, Pohang, South Korea.
Administrator of the cluster computer at MSE^2, MIT, Cambridge, USA.

3. Reviewer : Carbon, Physical Review B, ACS Fuel, J. Phys.: Condens Matter

4. Mobility :
One year at POSTECH, South Korea (APCTP : Asia Pacific Center for Theoretical Physics).
Third year at MIT, USA (MSE^2 : MultiScale Materials Science for Energy and Environment).

Teaching

2008-2011 : Teacher at the University of Cergy-Pontoise (200 hours).
Pedagogical manager of numerical simulations module. Each sessions was composed of a theoretical classes (2 hours), tutorials (4 hours) and practical work sessions (18 hours). I designed and wrote the manuscripts of courses, tutorials and practical work.

Tutorial of mechanics.

Practical work in programation (C++, python) and various numerical methods.

2015 : Teacher at the GDR MODMAT summer school at Istres, France (4 hours):
Modelization of carbon materials in interaction with metallic ones. This school aims to train Master 2 and PhD students, researcher and engineers from public and private companies who want to discover and/or going deeper in specific numerical techniques in simulated \ materials.

Industry

2017-2019 : TOTAL - project FASTER-SHALE : Thermodynamics and transport of alkanes in organic porous materials in geological conditions.

Rayonnement scientifique

1. Publications

20 articles in reviewed journals as : Science (IF 34.66), ACS Nano (IF 13.709), Physical Review Letter (IF 8.83), Nanoscale (IF 7.91), Carbon (IF 7.5), ...

2. International collaborations

(1) Department of Applied Physics, Aalto University School of Science, Puumiehenkuja 2, 00076, Aalto, Finland (H. Jiang, E. Kauppinen)
In situ monitoring of graphite damage by electronic irradiation.

(2) Graduate School of Natural Science and Technology, Okayama University, 3-1-1 Tsushima-naka, Kita-ku, Okayama 700-8530, Japan (I. Harada)
Spin transport in thin layers magnetic semiconductor by Monte Carlo simulations.

3. International conferences

2 Keynotes, 24 talks + 7 posters and 25 seminars.
Teacher at the summer school GDR MODMAT, Istres, France.

PhD at LPTM (Laboratoire de Physique Théorique et Modélisation, Cergy-Pontoise, november 2008/november 2011) :

Spin transport in thin layers magnetic semiconductor by Monte Carlo simulations.

Materials with a spontaneous magnetization undergo a transition from a magnetic phase (ferromagnetic, anti-ferromagnetic or frustrated) to a magnetic disorder phase (paramagnetic), depending on the temperature. For the past fifty years, the discovery of magnetic resistivity and the scattering mechanisms underlying the different behaviors of magnetic resistivity transitions near critical temperatures, figures 1A & 1B, has been controversial. Under the supervision of my PhD supervisor, we have developed a model capable of reproduce different experimental magnetic resistivity shown in Figure 1A. We also highlighted the different diffusion mechanisms according to the type of magnetism over a wide temperature range. This PhD work allows us to propose a unified spin transport model, capable of qualitatively and quantitatively reproduce the magnetic resistivities of many systems, particularly around transition temperatures. During my thesis, I developed several Monte Carlo Metropolis and Wang-Landau algorithms to carry out the different systems we focused on.

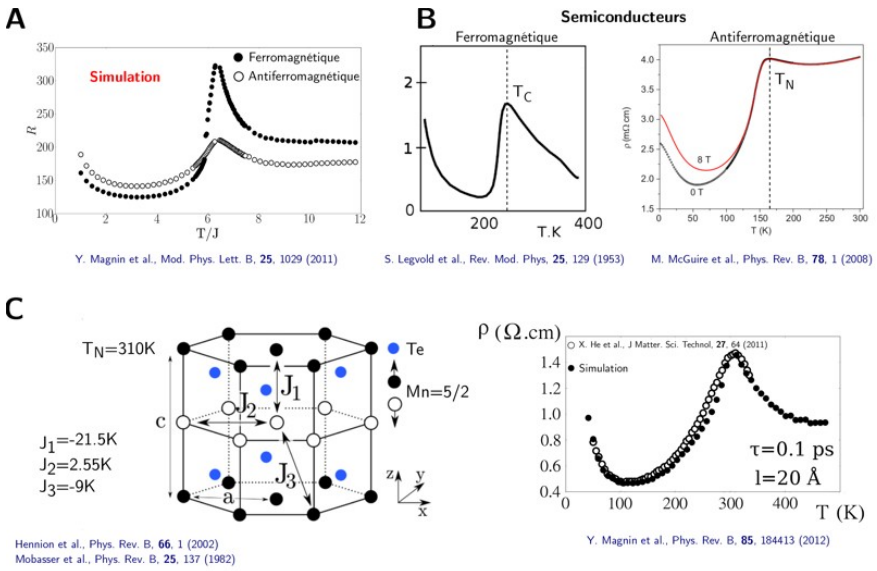

Figure 1 *– A. Simulation of magnetic resistivity (arbitrary unit) as a function of the temperature T for a ferromagnetic (black circles) and antiferromagnetic (white circles) semiconductor materials. B. Experimental magnetic resistivities as a function of T for a ferro and antiferromagnetic semiconductor. C. Simulation of the magnetic resistivity of MnTe alloy (circles black), experimental measurements (white circles).*

Postdoctorat at APCTP (Asia Pacific Center for Theoretical Physics, South Korea, november 2011/november 2012) :

Study of long range interactions accounting large dielectrical contrasts in the distribution of counter-ions on highly charged bio-molecule surfaces by finite elements.

The distribution of counter-ions on the surface of an highly charged bio-molecules (DNA, microtubules, ...) remains poorly understood theoretically. For systems composed of bio-molecules immersed in aqueous solution, counter-ions interact in an environment with an high dielectric contrast (Bio-molecule $\sim$ 2, Solvent $\sim$ 80). These systems present strong correlations capable to show attraction between bio-molecules with the same electrical charge. This phenomenon has been observed experimentally without having been clearly described by theory. The problem was studied on the basis of a field theory developed by Netz and Orland. This method consists to extract an Hamiltonian from the partition function of the system and to incorporate it into a Langevin equation in order to take into account correlations in the system. A finite element program coupled to a Runge-Kutta 4 algorithm was developed to determine distributions for different coupling regimes in Figure 2A. This approach allowed us to report the combined effects of strong coupling in an environment of high dielectric contrast. A depletion effect of counter-ions along the walls of bio-molecules was found on Figure 2B. This depletion originates a poor screening effect of the bio-molecules responsible of attraction. It should be noted, that the theoretical method used in this work is unstable for a large number of initial conditions.

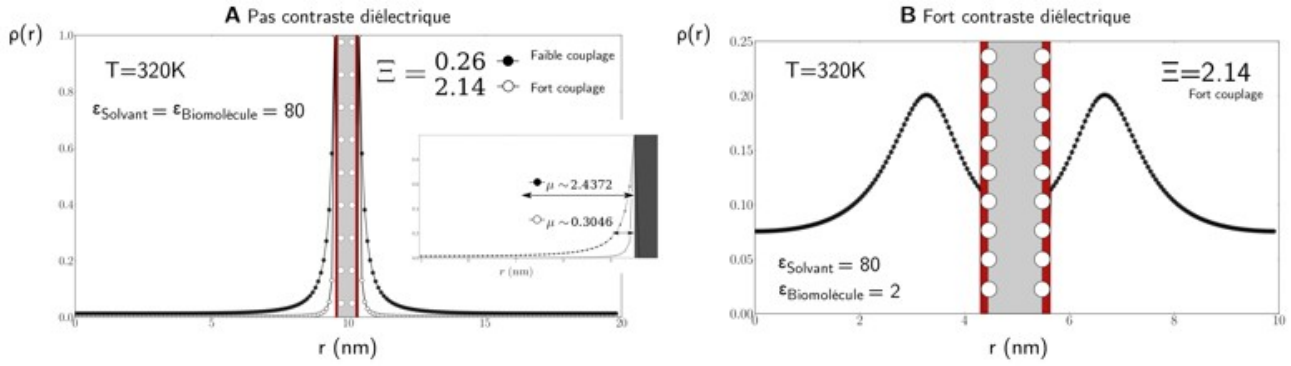

Figure 2 *– A. Density profile of counter-ions along the normal direction of the bio-molecule in a regime of low coupling (black circles) and high coupling (white circles) for an homogeneous dielectric environment. B. Density profile of counter-ions along the normal direction of the bio-molecule in highly coupled regime and in an environment of high dielectric contrast.*

Postdoctorat at ILM (Institut Lumière Matière, Lyon 1, january 2013/january 2014) :

Modelization of metallic nanoparticles supported on a graphene layer epitaxied on a metallic slab by Monte Carlo simulations.

Deposition of a graphene monolayer on certain transition metals of cubic crystallography offers perspectives for the nanostructuration of high-density magnetic storage materials. Structuration is possible thanks to the competition between the two immeasurable networks of the substrate (graphene/metal), giving rise to Moiré visible in electron microscopy, figure 3A. This work consisted in studying by numerical simulation the stability of nanoparticles deposited on an epitaxial graphene on metal figure3B. We began this work by evaluating carbon atomistic potentials proposed in the literature, in order to reproduce the structural properties of graphene. This first step of the work revealed a wide dispersion and qualitative disagreements depending on the potentials. a choice of potential was done by comparing the thermal expansion coefficients of graphene with each potentials that we cross-checked with experimental Raman spectroscopy measurements. The metal-substrate interactions were then parameterized from DFT data with the EAM functional to respect the respective symmetries of the graphene and the underlying metal. Our model allowed us to determine the equilibrium structures using Monte Carlo simulations in the isothermal-isobaric ensemble (NPT). Nanoparticle dynamics has been ensured by molecular dynamics simulation in the canonical ensemble (NVT).

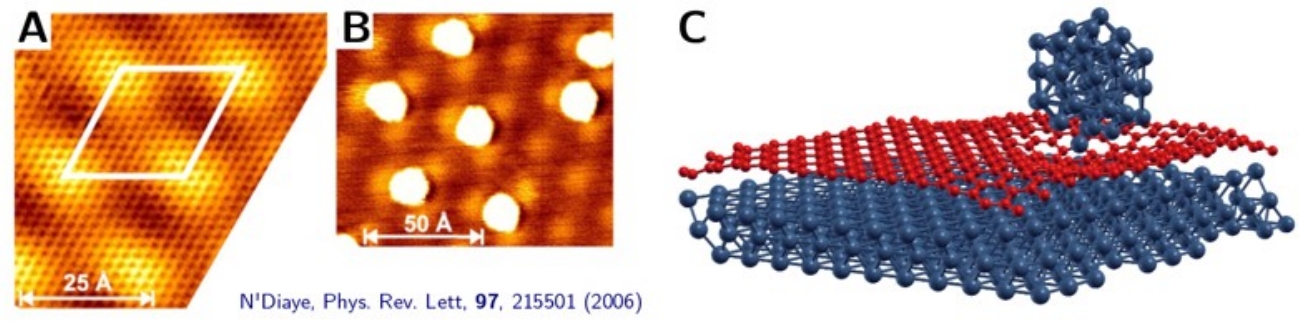

Figure 3 – *A. AFM images of a super moiré resulting from the interaction of two incommensurable lattices of graphene and metal. B. Self-organization of metallic nanoparticles deposited on the super moiré. C. Nanoparticle deposited on the moiré and relaxed by Monte Carlo simulation at finite temperature.*

Postdoctorat at CINaM (Centre Interdisciplinaire de Nanoscience de Marseille, january 2014/ september 2017) :

Nucleation and growth mechanisms of single wall carbon nanotubes by Monte Carlo simulations.

Carbon nanotubes offer an interesting alternative to replace critical metals such as indium oxide used in touch screens. However, the industrialization of carbon nanotubes is limited by a lack of control on the structural properties of the tubes during the synthesis. Indeed, no selective synthesis method is currently available to control the growth of tubes of given diameter, length and chirality. The synthesis of single-walled carbon nanotubes depends on the physico-chemical state of the catalyst where the nucleation then the growth occur. In the growth temperature range (900-1300 K), the catalyst (usually a transition metal nanoparticle as Ni, Co, Fe, Ag, ...) interacts with a carbon precursor and start to dissolve carbon atoms from this feedstock. Depending on the temperature, the chemical potential and the size of the nanoparticle, carbon atoms are adsorbed on the surface, diffuse to the sub-surface or in the core of the particle. Dissolved carbon atoms induce a particle transition from crystalline to a partial or a full liquid state. On the basis of Monte Carlo simulations using a Ni-C tight binding potential in the grand canonical ensemble, we have determined the Ni-C nanoparticle phase diagrams in typical thermodynamical growth condition. We have highlighted the evolution from a solid state to a disordered state of the catalyst through a continuum of core-shell states depending on their sizes. The calculated phase diagrams allowed us to highlight the diffusion and nucleation process of nanotubes. From these phase diagrams, we have shown that the control of the carbon concentration in the catalyst allows a selectivity in diameter and length of the tubes. These numerical predictions was latter confirmed experimentally. Finally, we have recently identified that the tube/catalyst interfacial binding energy is a key parameter to control the nanotube chirality. An analytical model allowing experimental predictions have been published in 2018 in the review Science.

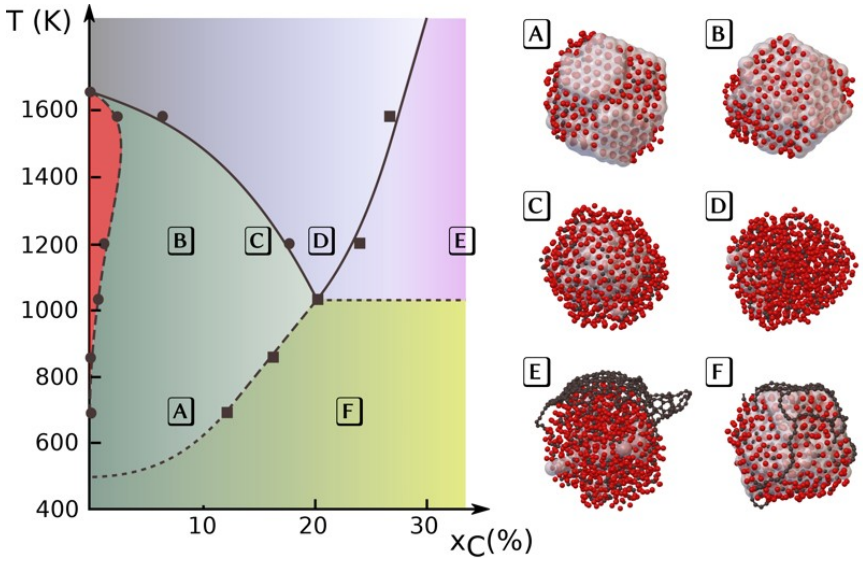

Figure 4 *– Ni-C phase diagram of a Wulff shape nanoparticle composed of 807 Ni atoms. The red domain corresponds to the solid state. The blue domain corresponds to the liquid state. The green domain correspond to the core-shell state composed of a crystalline core surrounding a disordered shell. At the right side of the solubility limit, the carbon segregation domain have two distinct phases, one liquid nanoparticle E and a core-shell nanoparticle F.*

Researcher scientist at MIT, <MSE^2> (Multiscale Material Science for Energy and Environment since September 2017) :

Atomistic simulations of metallic nanoparticles confined in porous carbon as CMK.

Less pollutant energy technology is a strategic challenge of our century. Hydrogen is one interesting candidate for energy production and storage. Hydrogen can be stored in a high pressure tank and more interestingly by physisorption in porous systems or by chemisorption in nanoparticle catalysts (NP). It has been shown that H isotherms depend on NP morphology that represent a poorly documented option to optimize H chemisorption. We show that wetting properties can be used to stabilized different NP morphologies when they are in contact with a carbon substrate. In case of a flat graphene, at low carbon concentration x_C~3%, the NP wets the substrate with a small metal/carbon interface. For carbon concentration corresponding a NP core-shell state x_C~10%, dissolved carbon atoms deplete the Ni layers at interface with the substrate (ordered Ni layers) and locate in the remaining volume of the NP (disordered Ni-C layers). Increase of x_C induces carbon diffusion from disordered to ordered layers, resulting in a gradual dewetting of the NP until detachment near carbon saturation x_C~25% for a Ni nanoparticle of few nanometers diameter (Figure 1).

We then study the effect of the substrate curvature on the wetting properties by using carbon nanotubes and CMK, a mesoporous carbon structure (Figure 2). We show that wetting properties of a core/shell nanoparticle are larger on a concave substrate than on flat or convex ones and is able to modify the NP morphology.

In this work, we show that the morphology of a nanoparticle can be control by two parameters: the carbon concentration dissolved inside the particle and the curvature which favores or defavores the metal/carbon interface formation at a constant x_C. Coupled effect of these two parameters allows to control the NP morphology from an spherical to a platelet shape.

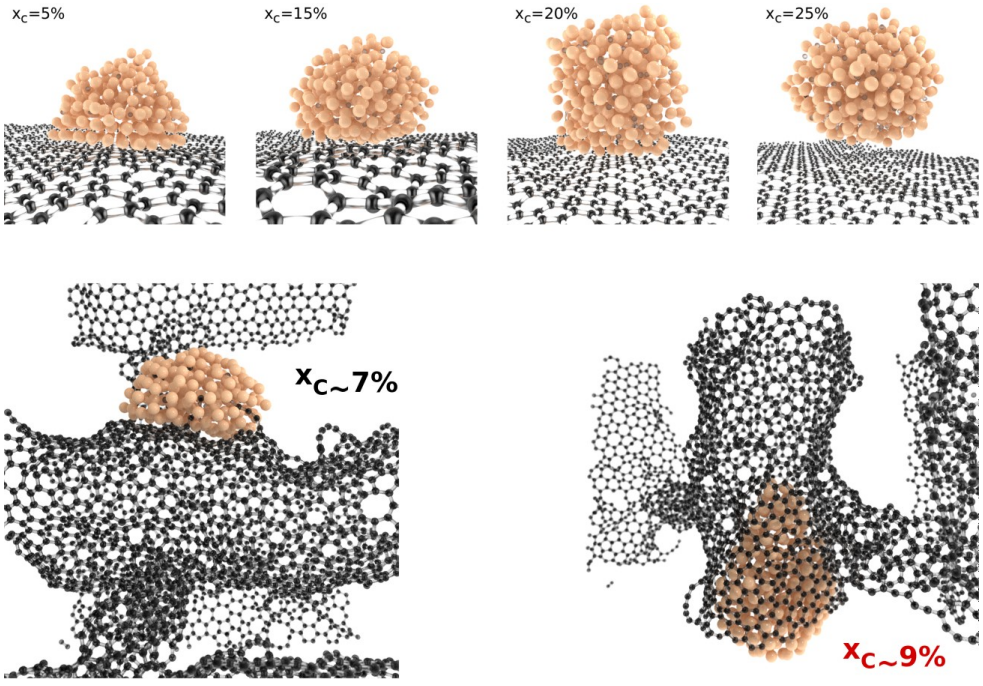

Figure 5 *– (Top) Wetting properties of a 201 Ni atoms nanoparticle supported on graphene as a function of the carbon concentration dissolved in it. (Bottom left), Wetting properties of a Ni-C nanoparticle on the convex surface of a mesoporous carbon structure CMK, spherical morphology. (Bottom right), Wetting properties of a Ni-C nanoparticle on the concave surface of a mesoporous carbon structure CMK, platelet morphology.*

Publications

[20] Morphology control of metallic nanoparticles supported on carbon substrates in catalytic conditions.
Y. Magnin, E. Villermaux, H. Amara, C. Bichara, R. Pellenq
Carbon **accepted** (2019)

[19] Cutting floating single-walled carbon nanotubes with a 'CO_2 blade'.
Y. Tian, N. Wei, P. Laiho, S. Ahmad, Y. Magnin, Y. Liao, C. Bichara, H. Jiang, E. Kauppinen
Carbon **143**, 481 (2019)

[18] Entropy driven stability of chiral single-walled carbon nanotubes.
Y. Magnin, H. Amara, F. Ducastelle, A. Loiseau, C. Bichara
Science **362**, 212 (2018)

[17] Growth Modes and Chiral Selectivity of Single-Walled Carbon Nanotubes.
M. He, Y. Magnin, H. Jiang, H. Amara, E. I. Kauppinen, A. Loiseau, C. Bichara
Nanoscale, **10**, 6744 (2018)

[16] Magnetism as indirect tool for carbon content assessment in nickel nanoparticles.
Y. Oumellal, Y. Magnin, A. Martinez de Yuso, J. M. Aguiar Hualde, H. Amara, V. Paul Boncour, C. Matei Ghimbeu, A. Malouche, C. Bichara, R. Pellenq, C. Zlotea
J. Appl. Phys. **128**, 213902 (2017)

[15] Structural Properties of Double-Walled Carbon Nanotubes driven by Mechanical Interlayer Coupling
A. Ghedjatti, Y. Magnin, F. Fossard, H. Amara and A. Loiseau
ACS Nano, **11**, 4840 (2017)

[14] Probing the role of carbon solubility in transition metal catalyzing single-walled carbon CNT growth.
J-M. Aguiar-Hualde, Y. Magnin, H. Amara, C. Bichara
Carbon **120,** 226 (2017)

[13] Dependence of Carbon Nanotube Length and Diameter on their Growth Modes
M. He, Y. Magnin, H. Amara, H. Jiang, F. Fossard, A. Castan, E. Kauppinen, A. Loiseau, C. Bichara
Carbon **113**, 231 (2017)

[12] Nuclear quantum effects on the thermal expansion coefficient of hexagonal boron nitride monolayer
F. Calvo and Y. Magnin
Eur. Phys. J. B **89**, 56 (2016)

[11] Size dependent phase diagrams of Nickel-Carbon nanoparticles
Y. Magnin, A. Zappelli, C. Bichara, H. Amara and F. Ducastelle
Phys. Rev. Lett. **115**, 205502 (2015)

[10] Interplay between Raman shift and thermal expansion in graphene: temperature-dependent measurements and analysis of substrate corrections
S. Linas, Y. Magnin, B. Poinsot, O. Boisron, G. D. Förster, Z. Han, D. Kalita, V. Bouchiat, V. Martinez, R. Fulcrand, F. Tournus, V. Dupuis, F. Rabilloud, L. Bardotti, F. Calvo
Phys. Rev. B **91**, 075426 (2015)

[9] Thermal expansion of freestanding graphene: benchmarking semiempirical potentials
Y. Magnin, G. D. Förster, F. Rabilloud, F. Calvo, A. Zappelli, C. Bichara
J. Phys.: Condens Matter **26**, 185401 (2014)

[8] Effective embedded-atom potential for metallic adsorbates on crystalline surfaces
G. D. Förster, Y. Magnin, F. Rabilloud, F. Calvo
Mod. Simul. Mater. Sci. Eng. **22**, 035015 (2014)

[7] Monte Carlo study of magnetic resistivity in semiconducting MnTe
Y. Magnin, H. T. Diep
Phys. Rev. B **85**, 184413 (2012)

[6] Spin resistivity in magnetic materials (Proceeding)
H. T. Diep, Y. Magnin and Danh-Tai Hoang
Acta. Phys. Pol. A **121**, 985 (2012)

[5] Spin Resistivity in Frustrated Antiferromagnets
Y. Magnin, K. Akabli, H. T. Diep and Isao Harada.
Phys. Rev. B **83**, 144406 (2011)

[4] Spin transport in magnetically ordered systems : effect of the lattice relaxation time (Proceeding)
Y. Magnin, Danh-Tai Hoang, Diep H. T.
Mod. Phys. Lett. B **25**, 1029 (2011)

[3] Monte Carlo Spin Transport in Antiferromagnetic Films: Application to MnTe
K. Akabli, Y. Magnin, H. T. Diep and Isao Harada
Phys. Rev. B **84**, 024428 (2011)

[2] Spin resistivity in the Frustrated J1-J2 Model (Proceeding)
Danh-Tai Hoang, Y. Magnin and H. T. Diep
Mod. Phys. Lett. B **25**, 937 (2011)

[1] Monte Carlo Study of the Spin Transport in Magnetic Materials
Y. Magnin, K. Akabli,H. T. Diep and Isao Harada
Comp. Mat. Sci. **49**, S204 (2010)

Conferences

[27] **Workshop TOTAL,** Annual meeting
Toronto, Canada, October 2019.
1 Talk

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[26] **CESEP'19,** 8th International conference on carbon for energy storage and environment protection.
Alicante, Spain, October 2019.
1 Talk

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[25] **Carbon conference,** The World conference on carbon
Lexington, USA, July 2019.
1 Keynote + 1 Talk

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[24] **GDRI M2UN,** Multi-scale Materials Under the Nanoscope.
Washington DC, USA, December 2018.
1 Talk

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[23] **Carbon conference**, The World conference on carbon
Madrid, Spain, July 2018.
1 Talk + 2 posters

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[22] **Workshop PyroMaN**, Annual meeting
Madrid, Spain, June 2018.
1 Talk

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[21] **Workshop TOTAL,** Annual meeting
Montreal, Canada, April 2018.
1 Talk

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[20] **SFEC,** French-Japanese Seminar on Carbon Materials.
Lyon, France, October 2017.
1 Talk

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[19] **CESEP'17**, 7th International conference on carbon for energy storage and environment protection.
Lyon, France, October 2017.
1 Talk

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[18] **SFEC**, Colloque Francophone du Carbone.
Saint Pierre d'Oléron, France, May 2017.
2 Talks

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[17] **GDRI M2UN**, Multi-scale Materials Under the Nanoscope.
Paris, France, December 2016.
1 Talk

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[16] **GDR-I GNT**, Graphene & Nanotubes: Science and applications.
Saint Pierre d'Oléron, France, October 2016.
1 Talk

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[15] **SFEC**: Colloque Francophone du Carbone.
Carqueiranne, France, May 2016.
1 Talk

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[14] **WORKSHOP MITSI**, Ecole supérieure d'Art d'Aix-en-Provence, "Esthétique des nanosciences",
Marseille, France, January 2016.
1 Talk

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[13] **GDR MODMAT**, Ecole d'été "Modélisation des Matériaux
Istres, France, July 2015.
1 Talk

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[12] **CECAM**, Modeling metal-based nanoparticles: toward realistic environments.
Toulouse, France, July 2015.
1 keynote

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[11] **GFEC**: Colloque Francophone du Carbone.
Les Karellis, France, Mai 2015.
1 Talk

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[10] **Guadalupe Workshop VII**, Nucleation & growth of SWCNT.
Rice University, Texas, USA, April 2015.
1 Poster

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[9] **GDR MODMAT**, 2ème réunion plénière
Lyon, France, Janvier 2015.
1 Talk

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[8] **Graphene and Nanotubes**: Science and Applications. Annual meeting of the GDR-I GNT
Strasbourg, France, September 2014.
1 Talk

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[7] **NT14**: The Fifteenth International Conference on the Science and Application of Nanotubes.
University of Southern California, Los Angeles, USA, June 2014.
1 Talk

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[6] Frontier Research in Graphene-based Systems (Graphene & Co).
Cargese, Corsica, April 2014.
1 Talk

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[5] 7th International Conference on Theory of Atomic & Molecular Clusters (TAMC VII).
University of Birmingham, UK, September 2013.
1 Poster

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[4] Workshop on Coulomb Many-body Systems.
Shanghai Jiao Tong University, Shanghai, China, July 2012.
1 Poster

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[3] The European Conference Physics of Magnetism 2011 (PM'11).
Institute of Molecular Physics, Poznan, Poland, June-July 2011.
1 Talk

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[2] International Conference on Frustrated Spin Systems, Cold Atoms and Nanomaterials.
Institute of Physics, Hanoi, Vietnam, July 2010.
1 Poster

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[1] 5th Conference of the Asian Consortium on Computational Materials Sciences (ACCMS-5).
Institute of Physics, Hanoi, Vietnam, September 2009.
1 Talk