## Emmanuel ARRAS

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# PhD Student
# Research Masters Degree in Condensed Matter and Radiation Physics

**Joseph Fourier University - Grenoble**

## *EDUCATION*

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|---|---|
| October 2006 : to February 2010 | PhD thesis in L_Sim (Atomistic simulation laboratory) in CEA – INAC – Grenoble<br>Numerical investigation of the atomic structure of germanium-manganese nanocolumns. Defense planned in February. |
| 2005 - 2006: | Research Master in Condensed Matter and Radiation Physics, graduated with honours (Université Joseph Fourier – Grenoble): Quantum Mecanics, Statistical Physics, Condensed matter Physics... |
| 2004 - 2005: | Master in Physics, graduated with honours (Université Joseph Fourier – Grenoble): Quantum Mecanics, Statistical Physics, Atomic and Subatomic Physics... |

## *RESEARCH EXPERIENCE*

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| October 2006 : to February 2010 | PhD thesis in L_Sim (Atomistic simulation laboratory) in CEA – INAC – Grenoble<br>Investigation of GeMn systems using ab-initio simulations and strong interactions with experiments. Simulation of magnetic, electronic and mechanical properties. |
| 2007-2009: | Teacher at IUT « Mesure Physique » (diploma in Technological sciences), Université Joseph Fourier<br>Mathematics (linear algebra, integrals,...: 21 hours/year) and Physics (electromagnetism: 42 hours/year) |
| March - July 2006: | Internship in L_Sim (Atomistic simulation laboratory) in CEA (INAC/SP2M/L_Sim) – Grenoble<br>Research work about vacancies and dopants in silicon: Numerical simulation by ab-initio methods of the migration of charged vacancies in silicon. |
| April - June 2005: | Internship in CRETA (Consortium de Recherches pour l'Émergence de Technologies Avancées) – CNRS – Grenoble<br>Research work on magnetic metals: Numerical simulation of the Ostwald ripening under strong magnetic fields. |

## *FOREIGN LANGUES AND COMPUTER SKILLS*

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| French: | native speaker |
| English: | fluent |
| German: | good skills, both written and spoken. |
| Operating systems: | Linux, Unix, Windows, Dos |
| Basic Softwares: | Maple, Mathematica, Matlab, AutoCad, Catia, 3ds Max |
| Langages: | C, Fortran, Python, shell, Pascal, Visual Basic, OpenGL |

## *ACTIVITIES AND INTERESTS*

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| Hobbies: | Alpine skiing and skitouring, climbing, mountain biking, rowing (silver and bronze medals in 2003 and 2004 during french university championship). |

## *REFERENCES*

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|---|---|
| Pascal POCHET | PhD supervisor – CEA Grenoble / L_Sim (pascal.pochet@cea.fr) |
| Thierry DEUTSCH | Head of L_Sim laboratory – CEA Grenoble / L_Sim (thierry.deutsch@cea.fr) |
| Eric BEAUGNON | Head of CRETA, Master trainee supervisor – CNRS Grenoble / CRETA (beaugnon@grenoble.cnrs.fr) |
| Marc TORRENT | Co-worker – CEA Bruyères-Le-Châtel / CEA-DAM (marc.torrent@cea.fr) |
| Matthieu JAMET | Head of Nanostrucures and Magnetism laboratory (NM) – CEA Grenoble / NM (matthieu.jamet@cea.fr) |

## *SCIENTIFIC WORKS*

**Simulations:**

- ab-initio:
  - Ground state: point defects in semiconductors (formation energy, charge and magnetic state, bond lenght, ...), phases (relative stability, phase diagram, interfaces, …).
  - Physical properties: phonon spectrum, structural, electronic and magnetic properties.
  - Out of equilibirum state: search for saddle point (NEB, DIIS), transition energy, metastability, phase segragation.
  - Strong method expertise: use of both norm conserving and PAW formalism, with pseudopotential generation for the latter. Participation to the implementation of non-colinear magnetism in the PAW formalism in Abinit. Use of different codes (mainly ABINIT, but also CPMD, SIESTA, PWSCF). Moderator on the Abinit Forum in the sections « Pseudopotentials » and « Structural Optimisation ».
- Diffraction simulation:
  - X-ray absorption spectroscopy (XANES and EXAFS).
  - Different codes used (Green's Functions method): FEFF (Atomic Sphere Approximation), FDMNES (finite difference).
- Monte Carlo: coding of a metropolis algorithm simulating the Ostwald ripening under strong magnetic fields.

**Experimental methods knowledges:**

- XANES, EXAFS, XMCD, Transmission Electron Microscopy, X-ray Diffraction, RBS channeling: instigation of an experiment (scheduled end of 2009). Strong interaction with experimentalists.

## *COMMUNICATIONS*

**Published Papers:**

« *Simulation of the enhanced Curie temperature in $Mn_5Ge_3C_x$ compounds* »
I. Slipukhina, E. Arras, P. Mavropoulos, and P. Pochet
Applied Physics Letters, Vol. **94**, p. 242510 (2009)

« *Atomic structure of Mn-rich nanocolumns probed by x-ray absorption spectroscopy* »
M. Rovezzi, T. Devillers, E. Arras , F. d'Acapito, A. Barski, M. Jamet, and P. Pochet
Applied Physics Letters, Vol. **92**, p. 242510 (2008)

« *Ostwald ripening in high magnetic field: analytical and numerical approach of polarized diffusion* »
E. Beaugnon, and E. Arras
Journal of Physics: Conference Series 51 (2006) 439–445

**Submitted papers:**

*« Metastability of $Ge_2Mn$ phase from first principle calculations »*
E. Arras, I. Slipukhina, M. Torrent, D. Caliste, T. Deutsch, and P. Pochet
submitted to Applied Physics Letters (October 2009)

**Papers under redaction:**

*« Atomic structure of Mn-rich nanocolumns: a combined computational and experimental study »*
E. Arras, I. Slipukhina, S. Tardif, M. Rovezzi, T. Devillers, M. Jamet, A. Barski, F. d'Acapito, S. Cherifi, J. Cibert, P. Bayle-Guillemaud, V. Favre-Nicolin, and P. Pochet
to be submitted to Nature Materials (spring of 2010)

*« First principle study of supersaturation and precipitation in GeMn »*
E. Arras, I. Slipukhina, D. Caliste, T. Deutsch, and P. Pochet
to be submitted to Physical Review B (spring of 2010)

**Patent (french):**

*« Matériau magnétique à base de semi-conducteur. »* (semiconductor based magnetic material)
P. Pochet, and E. Arras, submitted August 2008.

**Oral presentations:** « *Computational investigation of the atomic structure of Mn-rich nanocolumns »*

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| November 2009: | Scienomics Conference 2009, Paris, France, Invited Speaker<br>E. Arras, I. Slipukhina, T. Deutsch, and P. Pochet |
| April 2009: | MRS 2009, San Francisco, US<br>E. Arras, I. Slipukhina, T. Deutsch, and P. Pochet |
| March 2009: | Workshop developpeurs ABINIT, Autrans, France<br>E. Arras, I. Slipukhina, T. Deutsch, and P. Pochet |
| February 2009: | GDR DFT, Dourdan, France<br>E. Arras, T. Deutsch, and P. Pochet |
| January 2009: | GDR nanoalliage, Lyon, France<br>E. Arras, T. Deutsch, and P. Pochet |

**Posters:**

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| Nov. 2008: | « *Computational investigation of the atomic structure of Mn-rich nanocolumns: comparison with a possible GeMn ordered compounds* »<br>International Workshop Computational Magnetism and Spintronics, Dresde, Germany<br>E. Arras, I. Slipukhina, and P. Pochet |
| Nov. 2008: | « *Magnetic properties of $Mn_5Ge_3C_x$ compounds.* »<br>International Workshop Computational Magnetism and Spintronics, Dresde, Germany<br>I. Slipukhina, E. Arras, and P. Pochet |
| March. 2007: | « *DFT Study of charged vacancies and divacancies in silicon* » GDR DFT, Autrans, France<br>E. Arras, F. Lançon, T. Deutsch, P. Pochet |