Personal information

Surname(s) / First name(s)	**Hirel Pierre**
Address(es)	Unité Matériaux Et Transformations (UMET), Bâtiment C6, Université de Lille 1, 59655 Villeneuve d'Ascq, France
Telephone(s)	+33 3 20 43 48 61
Email(s)	pierre.hirel(at)univ-lille1.fr
Nationality(-ies)	French
Date of birth	17.11.1980
Gender	Male
Web page	http://pierrehirel.info/

Specialisation	**Research, simulations for materials physics**
Themes	Atomic-scale simulations, plasticity, dislocations, diffusion, complex materials
Current position	Post-doc, Université Lille, France

Competences

Simulation codes	***Ab initio* calculations** : VASP, Quantum Espresso, ABINIT, SIESTA **Atomistic simulations** : LAMMPS, XMD, GULP, DL_POLY
Codes developed	**Atomsk** (Web page)
Programming languages	Fortran 90/95, notions in C, shell (Windows, Unix/Linux), web (xhtml, php/MySQL)
Communication	LaTeX, LibreOffice, Scribus, Web (Dotclear, WordPress)
Spoken languages	**French** (mothertongue) **English** (TOEIC: 945, April 2008) **German** Beginner
Passions	Physics, computer science, cinema, piano.

Formation

2008-2009	Self-teaching of web languages: xhtml, css, php, W3C norms
Nov. 2008	**PhD in materials physics**, Univ. Poitiers. Very Honorable
June 2007	Summer school on *ab initio* code SIESTA, organized by CECAM (Lyon)
Déc. 2006	Course on parallel programming with Fortran/MPI, organized by IDRIS (Poitiers)
Jan.-June 2006	Course of history of sciences, Univ. Poitiers
June 2005	**Master of Sciences and Technologies**, Univ. Rennes1.
May-July 2003	**Internship in a company**, computer detailer AZERTY, Rennes Build, repair computers, install a system, set up networks...
Juin 2003	**Licence of Physique**, Univ. Rennes1.

Research

Since 1 Nov. 2012 — **Post-doc, UMET, Univ. Lille, France**

◇ Contribution to the RheoMan project (ERC Advanced Grant). Simulation of planar defects and dislocations in magnesium silicate perovskite $MgSiO_3$ in the conditions of Earth's mantle, by means of atomistic simulations (codes GULP, LAMMPS).

1er Feb. 2009 - 30 Sept. 2012 — **Post-doc, IAM-ZBS, Karlsruher Institut für Technologie, Germany**

◇ Simulation of planar defects and dislocations in functional perovskite materials ($SrTiO_3$, $KNbO_3$...), using *ab initio* calculations (code VASP) and atomistic methods (codes GULP, LAMMPS, DLPOLY). Collaboration with M. Mrovec, C. Elsässer (Fraunhofer-IWM, Freiburg, Germany) ; W. Sigle, P. van Aken, Max-Plank-Institut für Intelligente Systeme, Stuttgart (Germany).

Post-doc (invited researcher), Fraunhofer-IWM, Freiburg, Germany

◇ Study of the diffusion of Li^+ ions in new materials for Li-ion batteries. Collaboration with A. Hashibon, C. Elsässer (Fraunhofer-IWM, Germany) ; T. Eckl, U. Eisele (Robert Bosch GmbH, Germany) ; B. Kozinsky (Robert Bosch LLC, USA).

◇ Contribution to the european project RoLiCer : study of mechanical properties and the influence of dopants on fracture in Si_3N_4. Collaboration with european Universities and companies.

2008 — Co-organisation of a PhD student session in the conference C'NANO 2008

2005-2008 — **PhD Thesis, Laboratoire Phymat, Poitiers**

«Study by atomic-scale simulations of the formation of dislocation loops from surface ledges in a metal under stress»

Supervisors : S. Brochard, L. Pizzagalli, P. Beauchamp

◇ Characterisation of incipient plasticity in a metallic thin film, using atomic-scale simulations (codes XMD, LAMMPS). Derivation of a model based on elastic theory of dislocations. Development of a code (Fortran) for characterizing dislocations.

Jan.-June 2005 — **Research project, Master 2nd year, Laboratoire GMCM, Rennes**

«Theoretical study of electronic and optical properties of boron nnitride nanotubes»

Supervisor : B. Arnaud

◇ *Ab initio* calculations, using pseudopotentials (code ABINIT) or plane-waves (code PAW), of electronic band structures of hexagonal boron nitride (BN) and BN nanotubes, without and with excitonic corrections (GW approximation). Derivation of a tight-binding model. Simulation of optical spectra.

Jan.-June 2004 — **Research project, Master 1st year, Laboratoire GMCM, Rennes**

«Graphite and carbon nanotubes : introduction to electronic band structure calculations»

Supervisor : B. Arnaud

◇ *Ab initio* simulation of electronic band structures.

Teaching

Jan.-June 2006 — **Practical course, metallurgy (30h)**: 1st year, IUT Poitiers

◇ Thermal treatment, mechanical tests, materials fatigue.

Reviewer

Reviewer for peer-reviewed journals — Computational Materials Science
International Journal of Solids and Structures

Extra-professional activities

2006-2009 — Contribution to the Web site Spectrosciences.com. Science and technology awareness, writing of popularisation articles.

2007-2008 — President of the PhD student associaion AESM (Poitiers): organisation of a visit to the synchrotron SOLEIL, webmaster of the Web site

2007 — Contribution to ActionPLUS, promoting science towards high-school students.

2006 and 2007 — Contribution to the «fête de la science», Poitiers.