Natalio Mingo

LITEN/LCH, CEA-Grenoble, 17 r. des Martyrs, Grenoble 38000♦(33)4 3878 0160♦ natalio.mingo@cea.fr
http://www-drfmc.cea.fr/Images/Pisp/mningo/index_en.html

Summary of research interests

- Theory of thermal and electronic transport.
- Nanomaterials. Nanotechnology. Surface Science.
- Computational physics.

Professional experience

2006-present	permanent senior scientist, **CEA-Grenoble.**
2007-present	adjunct professor, **UC Santa Cruz.**
2002-2006:	staff scientist, **NASA-Ames Center for Nanotechnology**
1999-2002:	research scientist, **NASA-Ames research center**.
1998-1999:	postdoctoral European Union fellow, **Himeji Institute of Technology, Japan**.
1997:	visiting scholar, **Lawrence Berkeley National Laboratory**.

Education

2007:	**diplôme d'habilitation à diriger des recherches** (DHDR), U. Joseph Fourier, Grenoble.
1997:	**PhD, physics**, Universidad Autónoma de Madrid, Spain. *Summa cum Laude*. Outstanding Ph.D. Thesis Award for year 1997.
1993:	**MSc, physics,** Universidad Autónoma de Madrid, Spain.

Proposals funded and directed

- 2009-2012 (awarded): *Ab initio coupled charge and thermal transport in nanostructures,* PI. **Agence Nationale de la Récherche, France. 220K Euro**.
- 2008-2011 (awarded): *Computational modeling of novel nanostructured thermoelectric materials*. PI. **RTRA foundation, France. 148K Euro**.
- 2007-2010 (ongoing): *First-principles calculations of phonon thermal transport in bulk and nanostructured materials*. PI. **National Science Foundation, U.S.A.**
- 2007-2009 (ongoing): Nanothermoelectrics. **PI**. IRG from the **E.U. 80K Euro**.
- 2005: **subgroup leader** (supervising over one postdoc and one research scientist). Title: *Thermoelectric Nanowire Composites for Energy Efficient Refrigeration and Power Generation in Space Applications.* Agency: **NASA**.

- 2004-2005: **principal investigator**. Title: *Vertical surround gate transistors and non-volatile memories by computer aided design and experimental prototyping.* Agency: **NASA**. Amount: **$ 200K**.

- 2002-2003: **principal investigator**. Title: *Nanowire based thermoelectric refrigeration*. Agency: **NASA**. Amount: **$ 80K**.

Patents

N. Kobayashi, N. Mingo, M. Plissonnier, and A. Shakouri, "*Silicide nanoparticle in silicon germanium matrix nanocomposites for silicon compatible thermoelectric energy conversion*", (international patent filed, PCT/2008/001020, 11 July 2008.)

Awards

- European Union Postdoctoral Fellowship for researchers in Japan (1998-1999).
- Outstanding PhD Thesis award for year 1997, Universidad Autónoma de Madrid.
- PhD fellowship from the Ministry of Education of Spain (1994-1997).
- Postgraduate fellowship from the Autonomous University of Madrid (1993).
- Summer scholarship from the Foreign Ministry of Spain (1994).
- Summer ERASMUS-TEMPUS (EU) scholarship (1993).

Teaching and mentoring

- Course: "Thermal and thermoelectric transport in nanostructured materials", UC Santa Cruz, Fall 2008.
- Lecturer and co-organizer at the Spring School on "Thermics of Nanomaterials and Nanosystems", Cargèse, France, 2008.
- Course: "Nanoscale thermal and thermoelectric transport", UC Santa Cruz, Fall 2007.
- Course: "Energy transport at the nanoscale", CEA-Grenoble, October 2007.
- Postdoctoral adviser for: I. Savic (2007-present), S. Wang (2007-present).
- Mentor for graduate students: Ch. Bera (EC Paris), 2008-present;Y. Chalopin (EC Paris), summers 2007-2008; W. Zhang (Purdue University), summer and winter 2005; J. O'Keeffe (Stanford University): 2000-2004.
- Tutor at the St. Quentin College Program (Patten University) 2002.

Invited talks and research stays

- **Invited talk,** at Minatec Crossroads, Grenoble, 2008.
  First-principles thermal transport calculations.
- **Invited talk,** CECAM workshop on structural, electronic and transport properties of quantum wires, Lyon, 2008.
- **Invited talk**, MRS meeting, San Francisco, 2007.
- **Invited talk,** APS March meeting, Denver, 2007.
- **Invited talk,** CECAM workshop on inelastic effects in transport, Lyon 2006.
- **Colloquium of the Physics Department**, Univ. of California at Riverside, 2006.
  The flow of interacting phonons through nanowires, nanotubes, and molecular junctions.

- **Invited talk**, MRS meeting, Boston, 2004. *Thermal conductivity of nanowhiskers and nanowires: insights from theory.*
- **Invited talk**, at Nanoconduction Inc., 2005.
- **Invited seminar**, Lawrence Berkeley Laboratory, 1999. *Theory of Inelastic Scanning Tunneling Spectroscopy.*
- **Invited talk**, EMRS 1997 spring meeting, Strasbourg, France. *Theoretical study of electric field manipulation of adsorbates using a Scanning Tunneling Microscope.*
- **Visiting researcher**, Heyrovský Institute of Physical Chemistry, Czech Academy of Sciences, Prague, January-February 1996.
- **Visiting researcher**, Department of Physics, University of Wrocław, Poland, December 1995.

Synergistic Activities

- **Co-organizer** of symposium on first principles methods in nanoscale transport, JMC11, Strasbourg 2008.
- **Co-organizer** of "GDR nanothermique" meeting for French groups working on nanoscale thermal transport, with 30 participants, Grenoble, March 2008.

Non-degree certificates

- Polish language, Servicio de Idiomas, Univ. Autónoma de Madrid, 1991-3.
- Modern Standard Arabic, Servicio de Idiomas, Univ. Autónoma de Madrid, 1991-3.
- Classical Arabic (5 year), Darek Nyumba centre (University of Comillas), 1996.

Other activities

- Member of the Nishi-Harima amateur symphonic orchestra, Japan (1998-1999).
- Volunteer for Habitat for Humanity International, Honduras, November 2003.

References

Dr. Meyya Meyyappan
Director, NASA-Ames Center for Nanotechnology
M/S 229, Moffett Field, CA 94035
meyya@orbit.arc.nasa.gov, (650) 604-2616

Prof. D. A. Broido
Boston College.
Chestnut Hill, MA02467
Higgins 230C
broido@bc.edu, (617)-552-3348
FAX: (617) 552 8478.

Dr. Deepak Srivastava
NASA-Ames Research Center.
229-1 Moffett Field, CA 94035
dsrivastava@mail.arc.nasa.gov,
(650) 604 3486.

Dr. M. Salmeron
Lawrence Berkeley National Laboratory.
Materials Sciences Division, M/S 66-208
1 Cyclotron Road, Berkeley, CA 94720
salmeron@stm.lbl.gov , (510) 486 6230 or 6704.
FAX: (510) 486 6044.

Prof. F. Flores
Universidad Autónoma de Madrid, Spain.
Facultad de Ciencias, C-V
E-28049 Madrid, Spain
fernando.flores@uam.es,+34-1-497.50.43.

Prof. K. Makoshi
Himeji Institute of Technology, Japan.
3-2-1 Kouto, Kamigori-cho, Ako-gun,
Hyogo 678-1297, Japan
makoshi@sci.u-hyogo.ac.jp, +81-7915-8-0151.

Publications

In preparation

58. G. Pernot, M. Stoffel, I. Savic, A. Jacquot, J. Schumann, G. Savelli, A. Rastelli, O.G. Schmidt, J. M. Rampnoux, S. Dilhaire, M. Plissonnier, S. Wang, and N. Mingo, *Precise control of thermal conductivity at the nanoscale via individual phonon barriers.*

57. N. Mingo, K. Esfarjani, D. A. Broido, and D. A. Stewart, *"Cluster" isotope effects on phonon conduction: the case of graphene.*

56. S. Wang and N. Mingo, *Improved thermoelectric properties of Mg$_2$Si$_x$Ge$_y$Sn$_{1-x-y}$ nanoparticle in alloy materials.*

Book chapters

55. N. Mingo, to appear within the series "**Topics in Applied Physics**", **Springer (2009)**.
Phonon transport through nano-contacts by Green's function methods.

Journal articles:

54. D. A. Broido, N. Mingo, and D. A. Stewart, **IMECE 2008-67049 (2008)**.
Phonon thermal transport in bulk and nanostructured materials from first principles..

53. J. S. Heron, T. Fournier, N. Mingo, and O. Bourgeois, **Nano Letters (2009)**. **DOI:** 10.1021/nl803844j
Mesoscopic Size Effects on the Thermal Conductance of Silicon Nanowire.

52. Y. Chalopin, S. Volz, and N. Mingo, **Journal of Applied Physics**, accepted **(2009)**.
Interface heat transfer between crossing carbon nanotubes, and the thermal conductivity of nanotube pellets.

51. R. S. Prasher, X.J. Hu, Y. Chalopin, N. Mingo, K. Lofgreen, S. Volz, L. F. Cleri, and P. Keblinski, **Phys. Rev. Lett.**, 102, 105901 **(2009)**.
Turning carbon nanotubes from exceptional heat conductors into insulators.

50. N. Mingo, D. Hauser, N. P. Kobayashi, M. Plissonnier, and A. Shakouri, **Nano Letters** 9, 711 **(2009)**.
The nanoparticle in alloy approach to efficient thermoelectrics: silicides in SiGe..

49. S. Wang and N. Mingo, **Phys. Rev. B**, 79, 115316 **(2009)**.
Effects of interface roughness and superlattice period length on thermoelectric electron filtering.

48. D. A. Stewart, I. Savic, and N. Mingo, **Nano Letters**, 9, 81 **(2009)**.
First-Principles Calculation of the Magnitude of the Isotope Effect on Boron Nitride Nanotube Thermal Conductivity.

47. I. Savic, D. A. Stewart, and N. Mingo, **Physical Review B**, 78 235434 **(2008)**.
Thermal conduction mechanisms in boron nitride nanotubes: few-shell or all-shell?

46. I. Savic, N. Mingo, and D. A. Stewart, **Phys. Rev. Lett.** 101, 165502 **(2008)**.
Phonon transport in isotope-disordered carbon and boron-nitride nanotubes: is localization observable?

45. N. Mingo, D. A. Stewart, D. A. Broido, and D. Srivastava, **Phys. Rev. B** 77, 033418 **(2008)**.
Phonon transmission through defects in carbon nanotubes from first principles.

44. D. A. Broido, M. Malorny, G. Birner, Natalio Mingo, D. A. Stewart, **Appl. Phys. Lett.** 91, 231922 **(2007)**.
Intrinsic lattice thermal conductivity of semiconductors from first principles.

43. S. De Franceschi and N. Mingo, **Nature Nanotechnology** 2, 538 **(2007)**.
Cooling electrons one by one.

42. W. Zhang, N. Mingo, and T. S. Fisher, **Phys. Rev. B**, 76, 195429 **(2007)**.
Simulation of phonon transport across a non-polar nanowire junction using an atomistic Green's function method.

41. N. Mingo and D. A. Broido, **J. Appl. Phys.**, 101, 014322 **(2007).**
Thermoelectric power factor of nano-porous semiconductors.

40. J. H. Seol, A. L. Moore, S. K. Saha, F. Zhou, L. Shi, Q. Ye, R. Scheffler, N. Mingo, and T. Yamada, **J. Appl. Phys.** 101, 023706 **(2007)**.
Measurement and analysis of thermopower and electrical conductivity of an indium antimonide nanowire from a vapor-liquid-solid method.

39. W. Zhang, N. Mingo, and T. S. Fisher, **Numerical Heat Transfer**, 51, 333 **(2007).**
The Atomistic Green's Function Method: An Efficient Simulation Approach for Nanoscale Phonon Transport.

38. W. Zhang, N. Mingo, and T. S. Fisher, **Journal of Heat Transfer**, 129, 483, **(2007)**.
Simulation of interfacial phonon transport in Si-Ge heterostructures using an atomistic Green's function method.

37. D. A. Broido and N. Mingo, **Phys. Rev. B** 74, 195325 **(2006)**.
Theory of the thermoelectric power factor in nanowire nanocomposite matrix structures.

36. N. Mingo, **Phys. Rev. B,** 74, 125402 **(2006)**.
Anharmonic phonon transport through molecular-sized junctions.

35. N. Mingo and D. A. Broido, **Phys. Rev. Lett.** 95, 096105 **(2005)**.
Carbon nanotube ballistic thermal conductance, and its limits.

34. D. A. Broido, A. Ward, and N. Mingo, **Phys. Rev. B** 72, 014308 **(2005)**.
Lattice thermal conductivity of silicon from empirical interatomic potentials

33. N. Mingo and D. A. Broido, **Nano Letters** 5, 1221 **(2005)**.
Length dependence of carbon nanotube thermal conductivity, and the "problem of long waves".

32. N. Mingo and D. A. Broido, **Phys. Rev. Lett.** 93, 246106 **(2004)**.
Lattice thermal conductivity crossovers in semiconductor nanowires

31. N. Mingo, **Appl. Phys. Lett.** 85, 5986 **(2004)**.
Thermoelectric figure of merit of II-VI semiconducting nanowires

30. N. Mingo, **Appl. Phys. Lett.** 84, 2652 (**2004**).
Thermoelectric figure of merit and maximum power factor of III-V semiconducting nanowires

29. L. Shi., Q. Hao, Ch. Yu, N. Mingo, X. Kong, and Z. L. Wang, **Appl. Phys. Lett.** 84, 2638 (**2004**).
Thermal conductivities of individual tin dioxide nanobelts

28. N. Mingo, **Phys. Rev. B** 68, 113308 (**2003**).
Calculation of Si nanowire thermal conductivity using complete phonon dispersion relations

27. N. Mingo and Liu Yang, **Phys. Rev. B** 68, 245406 (**2003**); also **Phys. Rev. B** 70, 249901.
Phonon transport in nanowires coated with an amorphous material: an atomistic Green's function approach

26. N. Mingo, L. Yang, D. Li, and A. Majumdar, **Nano Letters** 3, 1713 (**2003**).
Predicting the thermal conductivity of Si and Ge nanowires

25. N. Mingo, Q. Hao, Ch. Yoon, and L. Shi, **IEEE-**nano proceedings, 2, 259 (**2003**).
Theoretical analysis of SnO_2 nanobelt thermal conductivity

24. C. W. Bauschlicher, A. Ricca, N. Mingo, and J. Lawson, **Chem. Phys. Lett.** 372 (**2003**) 723.
On the current flow for benzene-1,4-dithiol between two Au contacts

23. K. Makoshi, N. Mingo, **Surface Science**, 502-503 (**2002**) 34.
Theory of inelastic scanning tunneling spectroscopy

22. N. Mingo and Jie Han, **Phys. Rev. B (rapid communications)** , 64, 201401/1-4 (**2001**).
Conductance of metallic carbon nanotubes dipped into metal

21. N. Mingo, Liu Yang and Jie Han, **J. Phys. Chem. B**, 105, 11142 (**2001**).
Current induced forces upon atoms adsorbed on conducting carbon nanotubes

20. S. Tikhodeev, Mingo N., K. Makoshi, T. Mii, and H. Ueba, **Surf. Sci.** 493, 63 (**2001**).
Contribution to a theory of vibrational scanning tunneling spectroscopy of adsorbates. Nonequilibrium Green's function approach

19. K. Makoshi, N. Mingo, T. Mii, H. Ueba and S. Tikhodeev, **Surf. Sci.** 493, 71-77 (**2001**). *Theory of vibrational excitations of adsorbates by the scanning tunneling spectroscopy*

18. N. Mingo, Liu Yang, Jie Han and M.P.Anantram, **Phys. Stat. Sol. B**, 226, 79-85 (**2001**).
Resonant versus anti-resonant tunneling at carbon nanotube A-B-A heterostructures

17. N.Mingo, J.Han, M.P.Anantram and L.Yang, **Surf. Sci.**, 482-485, 1130-4 (**2001**).
Potential drop along carbon nanotube devices with current flow

16. N.Mingo, K.Makoshi, T.Mii and H.Ueba, **Surface Science** , 482-485, 96 (**2001**).
Theory of the relation between Inelastic Scanning Tunneling Spectroscopy of adsorbates and their vibrational deexcitation

15. N.Mingo and K.Makoshi, **Phys. Rev. Lett.** 84 (**2000**) 3694.
Calculation of the Inelastic Scanning Tunneling Image of Acetylene on Cu(100)

14. N. Mingo and K. Makoshi, **Applied Surface Science**,162-163(**2000**)227-232.
Calculation of Scanning Inelastic Tunneling Profiles of Adsorbates: acetylene on Cu(100)

13. N. Mingo and K. Makoshi, **Surface Science** 438(**1999**)261-270.,
Excitation of vibrational modes of adsorbates with the Scanning Tunneling Microscope: many orbital theory

12. L. Jurczyszyn, N. Mingo and F. Flores, **Surface Science**, Volumes 402-404, (**1998**) 459-463. *Influence of the atomic and electronic structure of the tip on STM images and STS spectra*

11. N. Mingo and F. Flores, **Thin Solid Films** 318 (**1998**), 69-72.
Theoretical study of the electric field manipulation of adsorbates using a Scanning Tunnelling Microscope

10. N. Mingo, M. Rose and M. Salmeron, **Journal of Surface Analysis**, Vol. 3, No. 2 (**1998**).
STM induced rotation of acetylene molecules adsorbed on Pd(111)

9. N. Mingo and F. Flores, **Surface Science**, volume 395, nos. 2 and 3 (**1998**).
Lateral forces and atomic desorption induced by the electric field created by STM tips on metal surfaces

8. A.L. Vazquez de Parga, O.S. Hernan, R. Miranda, A. Levy-Yeyati, N. Mingo and F. Flores, **Phys. Rev. Lett**., (**1998**), vol. 80 (no. 2) 357-60.
Electron resonances in sharp tips and their role in tunneling spectroscopy

7. L. Jurczyszyn, N. Mingo and F. Flores, **Czech. J. of Phys.** Vol 47 (**1997**), No.4 p.407-413.
The influence of the geometry of the tip on STM images

6. N. Mingo and Z. Knor, **Chemical Physics Letters** 263 (**1996**) 8.
Trigonal images of transition metal atoms adsorbed on transition metal FCC (111) surfaces and their availability for Scanning Tunneling Microscope

5. C.Sirvent, S.Vieira, L.Jurczyszyn, N.Mingo and F.Flores **Phys. Rev. B**, 53 (**1996**) 16086.
Conductance step for a single atom contact at the STM: noble and transition metals

4. L. Jurczyszyn, N. Mingo and F.Flores, **Mat. Sci. and Engeneering B** 37 (**1996**) 93.
Conductance Simulation through Single Atom Junctions at the Scanning Tunnelling Microscope

3. N. Mingo et al., **Phys. Rev. B**, 54 (**1996**) 2225.
Theory of the STM: Xe on Ni and Al

2. F.Flores, P.L.de Andres, F.J.Garcia-Vidal, L.Jurczyszyn, N.Mingo and R.Perez. **Progress in Surface Science**, Vol.48, Nos.1-4, pp27-38, **1995**.
Adsorption of noble gases on metal surfaces and the scanning tunneling microscope

1. N.Mingo, J.A.Porto and J.Sanchez-Dehesa, **Phys. Rev. B**, 50, 11884-11894 (**1994**).
Doping-profile effects on the tunneling times of electrons confined in double-barrier heterostructures