

ROBERTO CAR

Professor of Chemistry, Princeton University

Department of Chemistry and Princeton Institute for the Science and Technology of Materials
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Research Activity: Electronic structure and numerical simulation (classical and quantum) of condensed and molecular systems; disordered (amorphous and liquid) systems; surfaces; defects; clusters; nanostructures; phase transitions; organic and biological molecules; chemical reactions, quantum transport in nanostructures

Born: Trieste, Italy, 3 January 1947

Education: Politecnico di Milano (Milan Institute of Technology), Italy, Doctor Degree, Physics, 1971

Appointments:

2006-present Ralph W. Dorn *31 Professor in Chemistry, Princeton University
1999-present Professor, Department of Chemistry & PRISM
1991-1999 Professor, Department of Physics, University of Geneva, Switzerland;
Director, IRRMA, EPFL, Lausanne, Switzerland
1990-1991 Professor, Condensed Matter Physics Sector, Intl. School for Adv. Studies (SISSA), Trieste, Italy
1984-1990 Associate Professor, Condensed Matter Physics Sector, Intl. School for Adv. Studies (SISSA), Trieste, Italy
1981-1983 Postdoctoral Fellow, IBM T.J. Watson Research Center, Yorktown Heights
1977-1981 1st Assistant, Dept. of Physics, EPFL, Lausanne, Switzerland
1975-1976 Research Associate, Dept. of Physics, Politecnico di Milano, Italy
1973-1974 Research Fellow, Dept. of Physics, University of Milan, Italy

Honors:

2005 Doctor Degree Honoris Causa, University of Trieste, Italy, for his innovative role in computational physics and his extraordinary contributions to numerical simulation
1999 Fellow, American Physical Society
1995 A. Rahman Prize of the American Physical Society for Outstanding Achievement in Computational Physics Research
1994 Miller Professor, Department of Physics, University of California, Berkeley, 1994
1990 Hewlett-Packard Prize of the European Physical Society for Outstanding Achievement in Solid State Physics

Ten recent publications (from over 230 on refereed journals):

1. E. Prodan, R. Car, Tunneling Conductance of Amine-Linked Alkyl Chains, *Nanoletters* **8**, 1771 (2008)

2. J. Morrone, R. Car, Nuclear Quantum Effects in Water, *Phys. Rev. Lett.* **101**, 017801 (2008)
3. M. Koentopp, C. Chang, K. Burke, R. Car, Density Functional Calculations of Nanoscale Conductance, *J. Phys.-Cond. Matt.* **20**, 083203 (2008)
4. J.L. Li, R. Car, C. Tang, N. Wingreen, Hydrophobic interaction and hydrogen-bond network for a methane pair in liquid water, *PNAS* **104**, 2626 (2007)
5. E. Prodan, R. Car, dc conductance of molecular wires, *Phys. Rev. B* **76**, 115102 (2007)
6. M. Sharma, R. Resta, R. Car, Dipolar correlations and the dielectric permittivity of water, *Phys. Rev. Lett.* **98**, 247401 (2007)
7. Burke, K., R. Car, and R. Gebauer, Density functional theory of the electrical conductivity of molecular devices, *Phys. Rev. Lett.*, **94**(14), 146803 (2005)
8. Wang, X.F., S. Scandolo, and R. Car, Carbon phase diagram from ab initio molecular dynamics, *Phys. Rev. Lett.* **95**(18), 185701(2005)
9. Gebauer R, Car R, Current in open quantum systems, *Phys Rev Lett* **93** 160404 (2004)
10. Gebauer R, Car R, Kinetic theory of quantum transport at the nanoscale, *Phys Rev B* **70** 125324 (2004)

Collaborators:

K. Burke, University of California, Irvine; M.H. Cohen, Princeton and Rutgers; C. Dismukes, Princeton; I. Aksay, Princeton; R. Prud'homme, Princeton; N. Wingreen, Princeton; F. DeAngelis, University of Perugia, Italy; R. Gebauer, ICTP, Trieste; R. Resta, University of Trieste, Italy; S. Scandolo, ICTP, Trieste; E. Prodan, Yeshiva; G. Galli, University of California at Davis.

Students and Post-Docs (last 5 years):

Current: Wei Chen, Lin Lin, Zhaofeng Li, graduate students; Xifan Wu, Federico Zipoli, Yeohoon Yoon, post-doctoral associates. Former students: Joe Morrone, currently post-doc at Columbia University; Varhadarajan Srinivasan and Y. Kanai, currently post-docs at LBNL, Simone Piccinin, currently postdoc at the University of Sidney (Australia), Manu Sharma, Xiaofei Wang, and Yudong Wu, currently technical staff members at financial institutions. Former post-docs: E. Prodan, currently Assistant Professor at Yeshiva University, S. Zilberman, currently member of the technical staff in a high tech company in Israel, K. Kudin, currently member of the technical staff at the Shell Research Laboratory (Texas); Je Luen Li, currently member of the technical staff with Shaw Research (New York); F. DeAngelis, currently professor at the University of Perugia, Italy; R. Gebauer, currently member of the technical staff (condensed matter theory group) at the International Centre for Theoretical Physics (Trieste, Italy)

Ph.D. Advisor: O. Svelto

Post-doctoral Advisors: A. Baldereschi (EPFL, Switzerland); S.T. Pantelides (Vanderbilt University)