

CURRICULUM VITAE

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Education

Ph.D., Physics Department, University of Illinois at Urbana-Champaign, USA (1984)

M.S., Physics Department, University of Illinois at Urbana-Champaign, USA (1980)

Diploma in Physics, University of Athens (1973)

Research And Teaching Appointments

1998 - : Senior Researcher, TPCI, NHRF, Athens, Greece.

2001 - : Coactive Member of the Teaching Staff of the Hellenic Open University,
Greece.

1993 - 1998: Associate Researcher, TPCI, NHRF, Athens, Greece.

1987 - 1993: Assistant Researcher, TPCI, NHRF, Athens, Greece.

1984 - 1987: Postdoctoral Researcher, Institute of Electronic Structure and Laser,
Research Center of Crete, Greece.

1979 - 1983: Research Assistant, University of Illinois at Urbana-Champaign, USA.

1978 - 1979: Teaching Assistant, University of Illinois at Urbana-Champaign, USA.

1976 - 1977: Graduate Fellow, Nuclear Research Center "Democritus", Athens, Greece.

1974 - 1975: Research Center of National Defence, Greece.

1973 - 1974: Research Associate, Physics Laboratory of University of Athens, Greece

Main Research Interests

- Theoretical (computational): electronic structure of solids, clusters and atoms.
- Advancement of quantum mechanical methods.

External Funding

Coordinator or participant in various national and international research and educational projects in collaboration with academic and industrial organizations (National: PENED, ENTEP, ISTOS, PYTHAGORAS, ARISTEIA, KRIPIS, Ministry of Labor Seminars; International: NATO, AFOSR, ONR, IKYDA).

Conferences and Invited Talks

14 international and 17 Greek conferences, 14 invited talks.

Teaching Activities

- Scientific Computing Seminars: Numerical Analysis (TPCI, NRHF, 1990-1993).
- Undergraduate courses in: Theoretical Mechanics, Electromagnetic Theory, Relativity Theory, Waves and Radiation, Modern Physics (School of Physical Sciences, Hellenic Open University, 2001-).
- Supervision of two undergraduate students.
- Supervision of one Master's student.
- Supervision of four Ph.D. students (TPCI/NRHF); Partial Supervision: Three Member Committee of other Ph.D. students, Seven Member Committee of two Ph.D. students.
- Supervision of one post-doctoral researcher.

Honors and Awards

- National representative of Greece at the International Society for Theoretical Chemical Physics (1989-)
- NRC "DEMOKRITUS" Fellowship (1976-1978)

- Military service at the Research Center of National Defence, Greece (1974-1975)
- Greek Government Fellowship (1969-1973)
- Referee in international scientific journals

Professional Affiliations and Activities

Former Member of the Greek, USA, and UK Physical Societies.

Collaborations with Universities and Research Centers

- Naval Research Laboratory and George Mason University, USA
- University of Munich and University of Ulm, Germany
- University of Nanjing, P.R. China
- National Technical University of Athens, Greece
- University of Athens, Greece
- University of Patras, Greece,
- University of Thessaloniki, Greece,
- University of Ioannina, Greece

Collaborations with Industry / Companies

- Hellenic Petroleum S.A.
- Virtual Trip Ltd.

Book

"Handbook of Calculated Electron Momentum Distributions, Compton Profiles, and X-Ray Form Factors of Elemental Solids", N.I. Papanicolaou, N.C. Bacalis and D.A. Papaconstantopoulos, CRC Press, (1991).

Book Chapter

"Thermally Excited Lattice Solitons", N. Theodorakopoulos and N.C. Bacalis, Proton Transfer In Hydrogen Bonded Systems (Ed. T. Bountis), Plenum Press New York 1992 pp 131-137.

Selected Recent Publications

1. "Existence of He²⁻ negative ions with two remote electrons in antibonding orbitals, N.C. Bacalis, [J. Phys. B 33, 1415 \(2000\)](#)
2. "Transferable tight binding parameters for paramagnetic and ferromagnetic iron, N.C. Bacalis, D.A. Papaconstantopoulos, M.J. Mehl and M. Lach-hab, [Physica B 296, 125 \(2001\)](#)
3. "Description of the chemical reaction path in the HCO molecule: a combined configuration interaction and tight-binding approach", N.C. Bacalis, A. Metropoulos and D.A. Papaconstantopoulos, [Phys. Rev. A 71, 022707/1-10 \(2005\)](#)
4. "Analytic atomic wave functions of NMCSCF quality - and applications", Z. Xiong, M. Velgakis, N.C. Bacalis, [Int. J. Q. Chem. 104 418 \(2005\)](#)
5. "Inherent restrictions of the Hylleraas-Undheim-MacDonald higher roots, and minimization functionals at the excited states", N.C. Bacalis, Z. Xiong and D. Karaoulanis, [J. Comput. Meth. Sci. Eng. 8, 277 \(2008\)](#) (Category: Invited Paper)
6. "Minimization principle for non-degenerate excited states (independent of orthogonality to lower lying known approximants)", N.C. Bacalis, [J. Comput. Meth. Sci. Eng. 16, 253, \(2016\) DOI: 10.3233/JCM-160616](#)
7. "Correct small-truncated excited state wave functions obtained via minimization principle for excited states compared/opposed to Hylleraas-Undheim and McDonald higher 'roots' ", Z. Xiong, J. Zang, H.J. Liu, D. Karaoulanis, Q. Zhou, N.C. Bacalis, [J. Comput. Meth. Sci. Eng. vol. Preprint, no. Preprint, pp. 1-15, \(20 March 2017\) DOI: 10.3233/JCM-170722](#)