CURRICULUM VITAE

Naoum C. Bacalis

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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

2018: Director of Research, TPCI, NHRF, Athens, Greece.
1998 - 2018: Senior Researcher, TPCI, NHRF, Athens, Greece.
2001 - 2017: 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 Chapters

- "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.

- "If truncated wave functions of excited state energy saddle points are computed as energy minima, where is the saddle point?, N.C. Bacalis, Theoretical Chemistry for Advanced Nanomaterials - Functional Analysis by Computation and Experiment (Ed. T. Onishi), Springer Nature (to appear in 2019).

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, and N.C. Bacalis, J. Comput. Meth. Sci. Eng. vol. 17, no. 3, pp. 347-361, 2017 DOI: 10.3233/JCM-170722