# Naoum C. Bacalis

## ACADEMIC PUBLICATIONS

### 1.1 Books

"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).

### 1.2 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

### 1.3 In Refereed Journals

1. "Various Approximations made in Augmented Plane Wave Calculations", N.C. Bacalis, K. Blathras, P. Thomaides and D.A. Papaconstantopoulos , Phys. Rev. B 32, 4849 (1985)

2. "Ab initio Calculations of Selected Ionization States of Cu on MgO(001)", N.C. Bacalis and A.B. Kunz, Phys. Rev. B 32, 4857 (1985)

3. "Calculation of Compton Profiles of Tantalum and Tungsten", N.I Papanicolaou, N.C. Bacalis and D.A. Papaconstantopoulos , Phys. Status Solidi B 137, 597 (1986)

4. "Theoretical Compton Profiles Due to Valence-Electrons of Ti and $TiH_2$", N.C. Bacalis, N.I Papanicolaou, and D.A. Papaconstantopoulos , J. Phys. F-Met. Phys. 16, 1471 (1986)

5. "Calculation of the Compton Profiles of Vanadium, Niobium and Their Dihydrides", N.I Papanicolaou, N.C. Bacalis and D.A. Papaconstantopoulos , Z. Phys. B 65, 453 (1987)

6. "Exponential Tails in the Density of States", E.N. Economou, N.C. Bacalis and M.H. Cohen, J. Non-Cryst. Sol. 97, 101 (1987)

7. "Simple Derivation of Exponential Tails in the Density of States", N.C. Bacalis, E.N. Economou and M.H. Cohen, Phys. Rev. B 37, 2714 (1988)

8. "Tight-Binding Study of the Electron-Phonon Interaction in BCC Transition-Metals and Alloys", G. Fletcher, J.L. Fry, P.C. Pattnaik, D.A. Papaconstantopoulos and N.C. Bacalis, Phys. Rev. B 37, 4944 (1988)

9. "Calculation of the Electron Momentum Density in Zr and $ZrH_2$", N.I Papanicolaou, N.C. Bacalis and D.A. Papaconstantopoulos , Phys. Rev. B 37, 8627 (1988)

10. "Systematic Calculations of the Band Structures of the Rare-Gas Crystals Neon, Argon, Krypton, and Xenon", N.C. Bacalis, D.A. Papaconstantopoulos and W.E. Pickett, Phys. Rev. B 38, 6218 (1988)

11. "Band Structure and Electron-Phonon Interaction of $LaAgO_3$", N.C. Bacalis and D.A. Papaconstantopoulos , J. Superconductivity 1, 175 (1988)

12. "Excited Molecules and Clusters in Solid Media - Hydrogen and Tetrahydrogen in Ionic-Crystals", C.A. Nicolaides, P. Valtazanos and N.C. Bacalis, Chem. Phys. Lett. 151, 22 (1988)

13. "Directional and Two-dimensional Electron Momentum Density in Solid Vanadium", N.C. Bacalis and N.I. Papanicolaou , Studies In Physical And Theoretical Chemistry 62, 505, (1989)

14. "Theoretical Compton Profile of $ZrH_2$", N.I. Papanicolaou and N.C. Bacalis, Z. Phys. Chem. Neue Folge 163, 561 (1989)

15. "Comparison of the Electron Momentum and 2-Photon Momentum Distributions in Titanium and Zirconium Dihydrides", N.C. Bacalis, N.I. Papanicolaou and D.A. Papaconstantopoulos , Z. Phys. Chem. Neue Folge 163, 555 (1989)

16. "Ab-Initio Calculations on the Adsorption of H, O, and CO Atop Cu-2+ on MgO(001)", N.C. Bacalis and A.B. Kunz , Phys. Status Solidi B 156, 545 (1989)

17. "Electron Momentum Distribution and Compton Profiles of Crystalline Rare-Gases by the Augmented-Plane-Wave Method", N.C. Bacalis and N.I. Papanicolaou , Phys. Status Solidi B 157, 293 (1990)

18. "Total-Energy Calculations of Solid H, Li, Na, K, Rb, and Cs", M. Sigalas, N.C. Bacalis, D.A. Papaconstantopoulos, M.J. Mehl and A.C. Switendick , Phys. Rev. B 42, 1637 (1990)

19. "Hydrogen Molecule and Tetrahydrogen Cluster Embedded in Ionic-Crystals", P. Valtazanos, N.C. Bacalis and C.A. Nicolaides , Chem. Phys. 144, 363 (1990)

20. "Electron Momentum Distribution in Silver", N.I. Papanicolaou and N.C. Bacalis, Soc. It. Fisica 25, 211 (1990)

21. "Semiclassical Solitons and the S = 1/2 Heisenberg-Model", N. Theodorakopoulos and N.C. Bacalis , Phys. Rev. Lett. 67, 3018 (1991)

22. "Calculation of the Electron Momentum Density and Compton-Scattering Measurements for Nickel", D.L. Anastassopoulos, G.D. Priftis, N.I Papanicolaou, N.C. Bacalis and D.A. Papaconstantopoulos , J. Phys.: Condens. Matter 3, 1099 (1991).

23. "Total Energy and Band-Structure of the 3D, 4D, and 5D Metals", M. Sigalas, D.A. Papaconstantopoulos and N.C. Bacalis, Phys. Rev. B 45, 5777 (1992)

24. "Thermal Solitons in the Toda Chain", N. Theodorakopoulos and N.C. Bacalis, Phys. Rev. B 46, 10706 (1992)

25. "Theory for the Direct Construction of Diabatic States and Application to the $He_2^{(2+)}$ $^2\Sigma_g^{(+)}$ Spectrum", C.A. Nicolaides, N.C. Bacalis and Y. Komninos , Chem. Phys. Lett. 192, 486 (1992)

26. "State-Specific Theory and Method for the Computation of Diatomic-Molecules - Application to $He_2^{(2+)}$ $^1\Sigma_g^{(+)}$", N.C. Bacalis, Y. Komninos and C.A. Nicolaides, Phys. Rev. A 45, 2701 (1992) DOI:10.1103/PhysRevA.45.2701

27. "Lowest $^{(3)}\Delta_{(u)}$ State of $He_2$", N.C. Bacalis, Phys. Rev. A 47, 5206 (1993)

28. "Toward the Understanding of $He_2^{(-)}$ Excited-States", N.C. Bacalis, Y. Komninos and C.A. Nicolaides, Chem. Phys. Lett. 240, 172 (1995)

29. "Thermodynamics of the Ishimori-Haldane-Faddeev Ferromagnetic Chain - The Field-Dependent Case", N. Theodorakopoulos, N.C. Bacalis and Z. Xiong , Phys. Rev. B 54, 4033 (1996)

30. "Neutral Parent States of the Ionic $He_2^{(-)}$ $^{(4)}\Phi_{(g)}$", N.C. Bacalis, Phys. Rev. A 53, 3057 (1996) DOI:10.1103/PhysRevA.53.3057

31. "Variational Predictability of Diabatic, Adiabatic or Impossible Diatomic States", N.C. Bacalis, J. Phys. B: At. Mol. Opt. Phys. 29, 1587 (1996) http://dx.doi.org/10.1088/0953-4075/29/9/006

32. "Biomonitoring Human Exposure to Environmental Carcinogenic Chemicals", P.B. Farmer, O. Sepai, R. Lawrence, H. Autrup, P.S. Nielsen, A.B. Vestergard, R. Waters, C. Leuratti, N.J. Jones, J. Stone, R.A. Baan, J.H.M. Vandelft, M.J.S.T. Steenwinkel, S.A. Kyrtopoulos, V.L. Souliotis, N, Theodorakopoulos, N.C. Bacalis, A.T. Natarajan, A.D. Tates, A. Haugen, A. Andreassen, S. Ovrebo, D.E.G. Shuker, K.S. Amaning, A. Schouft, A. Ellul, R.C. Garner, K.H. Dingley, A. Abbondandolo, F. Merlo, J. Cole, K. Aldrich, D. Beare, E. Capulas, G. Rowley, A.P.W. Waugh, A.C. Povey, K. Haque, M. Kirschvolders, P. Vanhummelen, and P. Castelain, , Mutagenesis 11, 363 (1996)

33. "Low-Temperature Asymptotics of Isotropic Ferromagnetic Chains at Nonzero Fields", N. Theodorakopoulos and N.C. Bacalis, Phys. Rev. B 55, 52 (1997)

34. "Electronic-Structure of Ordered and Disordered Cu-Ag Alloys", N.C. Bacalis, G.F. Anagnostopoulos, N.I Papanicolaou and D.A. Papaconstantopoulos , Phys. Rev. B 55, 2144 (1997)

35. "Wave-Vector-Dependent Stoner Approach to Band Ferromagnetism in Ni", N.C. Bacalis, N. Theodorakopoulos and D.A. Papaconstantopoulos , Phys. Rev. B 55, 11391 (1997)

36. "Existence Of $He_2$- Negative Ions With Two Remote Electrons In Antibonding Orbitals", N.C. Bacalis, J. Phys. B: At. Mol. Opt. Phys. 33, 1415 (2000) http://dx.doi.org/10.1088/0953-4075/33/7/309

37. "Determination Of Working Length In Endodontic Therapy: How Accurately Can It Be Achieved With Current Methods?", J. Margelos, N.C. Bacalis and S. Perdicouris , Stoma 28, 39 (2000)

38. "Comment on the Formation of $He_2^-$ $^4I_g$ states", N.C. Bacalis, Chem. Phys. Lett. 331, 323 (2000)

39. "Interpretation Of The Spin Glass Behaviour Of Dilute Magnetic Semiconductors", D. Karaoulanis, J.P. Xanthakis and N.C. Bacalis, J. Mag. Mag. Materials 221, 407 (2000)

40. "Transferable Tight Bibding Parameters for Paramagnetic and Ferromagnetic Iron", N.C. Bacalis, D.A. Papaconstantopoulos, M.J. Mehl and M. Lach-hab , Physica B 296, 125 (2001)

41. "Applications of the NRL-TB method to magnetic systems", M.J. Mehl, D.A. Papaconstantopoulos, I.I. Mazin, N.C. Bacalis and W.E. Pickett , J. Appl. Phys. 89, 6880 (2001)

42. "Electronic apex locators: Operation principles and clinical considerations", J. Margelos, N.C. Bacalis and S. Perdicouris, Odontostomatological Progress 55, 187 (2001)

43. "Generalization of Laguerre orbitals toward an accurate, concise and practical analytic atomic wave function", Z. Xiong and N.C. Bacalis, MATCH Commun. Math. Comput. Chem. 53, 283 (2005)

44. "Analytic atomic wave functions of NMCSCF quality – and applications", Z. Xiong, M. Velgakis and N.C. Bacalis , Int. J. Q. Chem. 104, 418 (2005) DOI: 10.1002/qua.20638

45. "Description of the lowest-energy surface of the CH + O system: Interpolation of ab initio configuration-interaction total energies by a tight - binding Hamiltonian", N.C. Bacalis, A. Metropoulos and D.A. Papaconstantopoulos, Phys. Rev. A 71, 022707/1-10 (2005) DOI: 10.1103/PhysRevA.71.022707

46. "Analytic variationally optimized internally orthogonalized modified Laguerre orbitals in accurate atomic configuration interaction calculation", Z. Xiong and N.C. Bacalis, Chinese Phys. 15, 992 (2006) DOI: 10.1088/1009-1963/15/5/021

47. "Radiative decay from doubly to singly excited states of He via generalization of Laguerre type orbitals- A non-orthogonal formalism", Z. Xiong and N.C. Bacalis , Chinese Phys. 16, 374 (2007) DOI: 10.1088/1009-1963/16/2/017

48. "Interaction of Dioxygen with Al Clusters and Al(111): A Comparative Theoretical Study", C. Mosch, C. Koukounas, N.C. Bacalis, A. Metropoulos, A. Gross and A. Mavridis,, J. Phys. Chem. C 112, 6924 (2008), DOI: 10.1021/jp711991b

49. "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) DOI: http://iospress.metapress.com/content/9270636750564km0/ (Invited Paper)

50. "Properties of hydrogen terminated silicon nanocrystals via a transferable tight-binding Hamiltonian, based on ab-initio results", N.C. Bacalis and A.D. Zdetsis, J. Math. Chem. 46, 962 (2009) DOI: 10.1007/s10910-009-9557-x

51. "A generic procedure for determining atomic LS spectral terms and their LS eigenfunctions", Z. Xiong and N.C. Bacalis , Chinese Physics B 18, 542 (2009) DOI: 10.1088/1674-1056/18/2/026

52. "Shape of the Geometrically Active Atomic States of Carbon", Z. Xiong and N.C. Bacalis, Chinese Physics B 19, 023601 (2010) DOI:10.1088/1674-1056/19/2/023601

53. "Theoretical investigation of the interaction of $CH_4$ with $Al_2$ and $Al_3$ neutral and charged clusters" E.I. Alexandrou, A. Gross, and N.C. Bacalis, J. Chem. Phys. 132, 154701 (2010) DOI: 10.1063/1.3376174

54. "Theoretical Study of the $O_2$ Interaction with a Tetrahedral $Al_4$ Cluster", N.C. Bacalis, A. Metropoulos, and A. Gross, J. Phys. Chem. A 114, 11746 (2010) DOI: 10.1021/jp1052198

55. "Theoretical Study of the O2 + Al4 (Tetrahedral) System in Its Singlet State and Comparisons with Its Triplet State", N.C. Bacalis, A. Metropoulos, and A. Gross, J. Phys. Chem. C, 116, 16430 (2012) DOI: http://dx.doi.org/10.1021/jp3014833

56. "Accuracy study for excited atoms (ions): A new variational method", Z. Xiong, Z.-X. Wang and N.C. Bacalis, Acta Phys. Sin. 63, 053104, (2014) DOI: 10.7498/aps.63.053104.

57. "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.

58. "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. Preprint, no. Preprint, pp. 1-15, (20 March 2017) DOI: 10.3233/JCM-170722

## 1.4 In Refereed Proceedings of International Conferences

59. "Electrical Characterization of Gold-Tantalum GaAs Schottky Diodes using I-V and DLTS Measurements", G. Pananakakis, N.C. Bacalis, P. Panayotatos, G. Kiriakidis, and A. Christou. *Inst. Phys. Conf. Ser*. 91, 1988, pp 825-826

60. "Generalization of Laguerre orbitals toward an accurate, concise and practical analytic atomic wave function", Z. Xiong and N.C. Bacalis, *Proc. Int. Conf. Computational Methods In Sci. and Eng.* 2003, pp 687-691

61. "Lowest Energy Path of Oxygen near CH: A Combined Configuration Interaction and Tight-Binding Approach", N.C. Bacalis, A. Metropoulos and D.A. Papaconstantopoulos, *Lect. Ser. On Computer and Computational Sci.*, Brill Academic Publishers 1, 2004, pp 1015-1021

62. "Properties of silicon nanocrystals via a transferable tight-binding Hamiltonian, based on ab-initio results", A.D. Zdetsis and N.C. Bacalis; Lecture Series on Computer and Computational Science, Brill Academic Publishers, T. Simos and G. Maroulis (Eds.), vol. 4, pp. 1477-1479 (2005).

63. "Utilizing the fact that among all trial functions orthogonal to an approximate ground state, $\Phi^0$, the closest, $\Phi^{1+}$, to the exact first excited state,$\psi^1$, has lower energy than the exact: $E[\Phi^{1+}] < E[\psi^1]$", N.C. Bacalis; Proc. of the International Conference on Computational Methods in Science and Engineering 2007. Computation in Modern Science and Engineering, T.E. Simos and G. Maroulis (Eds.), AIP CP 963, vol. 2 Part A, pp. 6-9 (2007).

64. "Remarks on the Hylleraas-Undheim and MacDonald higher roots, and functionals having local minimum at the excited states", N.C. Bacalis, Z. Xiong and D. Karaoulanis, Proceedings of the ICCMSE-2008, 25-30 September 2008, Hersonissos, Crete, Greece; Computational Methods in Science and Engineering, Advances in Computational Science, AIP-CP1148, Vol. 2, pp. 372-375 (2009).

65. "Theoretical investigation of the interaction of $CH_4$ with $Al_n$ neutral and charged clusters", E.I. Alexandrou and N.C. Bacalis; Proceedings of the ICCMSE-2008, 25-30 September 2008, Hersonissos, Crete, Greece; Computational Methods in Science and Engineering, Advances in Computational Science, AIP-CP1148, Vol. 2, pp. 380-383 (2009).

66. "The Need, Benefits, and Demonstration of a Minimization Principle for Excited States", N.C. Bacalis; Proceedings of the ICCMSE-2015, 21-23 March 2015, Athens, Greece; Computational Methods in Science and Engineering, Advances in Computational Science, AIP- Conference Proceedings 1702 , 090008, **(**2015) DOI: 10.1063/1.4938816

67. "Computing Correct Truncated Excited State Wavefunctions", N.C. Bacalis, Z. Xiong, J, Zang, D. Karaoulanis, AIP Conference Proceedings 1790 **,** UNSP 020007, (2016), DOI: 10.1063/1.4968633

## 1.5 Other Publications (Proceedings of National Conferences, Techn. Journals etc.)

1. "Calculation of the electron momentum density and the Compton profile of the transition metals V(B) and their hydrides", N.C. Bacalis, N.I. Papanicolaou and D.A. Papaconstantopoulos, *Proc. II Greek Conf. on Solid State Physics*, Ioannina, 1986, p. 63 (in Greek).

2. "Electronic properties of superlattices and heterojunctions GaAs-$Ga_{1-x}Al_xAs$", A. Christou, G. Pananakakis, N. Bacalis, A. Ginoudi, *Proc. II Greek Conf. on Solid State Physics*, Ioannina, 1986, p. 59 (in Greek).

3. "Electron momentun distribution of Zr και $ZrH_2$", N.I. Papanicolaou, N.C. Bacalis and D.A. Papaconstantopoulos, *Proc. II Greek Conf. on Solid State Physics*, Ioannina, 1986, p. 53 (in Greek).

4. "Effects of the substutution of Cu by Ag in high $T_c$ Perovskites $LaCuO_3$" N.C. Bacalis and D.A. Papaconstantopoulos, *Proc. III Greek Conf. on Solid State Physics*, Patra, 1987, p. 41-43 (in Greek).

5. "Computation of electronic band structure, electron momentum distribution and Compton profiles of crystalline rare gases", N.C. Bacalis, D.A. Papaconstantopoulos, W.E. Pickett and N.I. Papanicolaou, *Proc. III Greek Conf. on Solid State Physics*, Patra, 1987, p. 62-64 (in Greek).

6. "Study of the energy states of Schottky diodes with Au-Ta on nGaAs", G. Pananakakis, N.C. Bacalis, P. Panagiotatos andA. Christou, *Proc. III Greek Conf. on Solid State Physics*, Patra, 1987, p. 139-140 (in Greek).

7. "Electron momentum density of Ag", N.I. Papanicolaou and N.C. Bacalis, *Proc. IV Greek Conf. on Solid State Physics*, Athens, 1988, p. 443-446 (in Greek).

8. "Seven-hydrogen clusters in hydrogenated Si", N.C. Bacalis, *Proc. IV Greek Conf. on Solid State Physics*, Athens, 1988, p. 447-449 (in Greek).

9. "One- and two-dimensional electron momentum density in crystalline Vanadium", N.C. Bacalis and N.I. Papanicolaou, *Proc. IV Greek Conf. on Solid State Physics*, Athens, 1988, p. 450-453 (in Greek).

10. "CI calculations in diatomic and tetratomic hydrogen clusters in NaCl-like charge arrays", P. Valtazanos, N.C. Bacalis and C.A. Nicolaides, *Proc. IV Greek Conf. on Solid State Physics*, Athens, 1988, p. 454-457 (in Greek).

11. "$H_2$ and $H_4$ embedded in NaCl type solids", P. Valtazanos, N.C. Bacalis*, and C.A. Nicolaides, 9th General Conference of the Condensed Matter Division of the E.P.S. Nice, France, 6-9 March 1989 (abstract).

12. "Computation of electron momentum density and spin-polarized Compton profile of ferromagnetic Ni", N.C. Bacalis, N.I. Papanicolaou and D.A. Papaconstantopoulos, *Proc. VI Greek Conf. on Solid State Physics*, Heraklion, 1990, p. 35-40 (in Greek).

13. "Solitons and thermodynamics of an integrable magnetic system", N. Theodorakopoulos and N.C. Bacalis, *Proc. VI Greek Conf. on Solid State Physics*, Heraklion, 1990, p. 182-185 (in Greek).

14. "Calculation of the total energy of H, Li, Na, K, Rb, and Cs solids", M. Sigalas, N.C. Bacalis, D.A. Papaconstantopoulos and A.C. Switendick, *Proc. VII Greek Conf. on Solid State Physics*, Thessaloniki, 1991, p. 36-39 (in Greek).

15. "Thermal solitons in the Toda plane", N. Theodorakopoulos and N.C. Bacalis, *Proc. VII Greek Conf. on Solid State Physics*, Thessaloniki, 1991, p. 190-196 (in Greek).

16. "Computation of electronic properties of $Pd_xAg_{1-x}$ alloys within the coherent potential approximation", G.F. Anagnostopoulos, N.I. Papanicolaou, N.C. Bacalis and D.A. Papaconstantopoulos, *Proc. IX Greek Conf. on Solid State Physics*, Patra, 1992, p. 286-289 (in Greek).

17. "Study of the electronic structure of $Cu_xAu_{1-x}$ alloys within the coherent potential approximation", N.I. Papanicolaou, N.C. Bacalis and D.A. Papaconstantopoulos, *Proc. X Greek Conf. on Solid State Physics*, Delphi, 1992, p. 286-289 (in Greek).

18. "State specific theory and computations of diatomic molecules", N.C. Bacalis*, Y. Komninos, and C.A. Nicolaides, Sanibel Symposium 1993, St. Augustine, Florida, USA, 13-20 March 1993 (abstract).

19. "A systematic study of the electronic structure of Cu-Au alloys with the tight-binding coherent-potential approximation", N.I. Papanicolaou*, N.C. Bacalis and D.A. Papaconstantopoulos, European Research Conference, Electronic Structure of Solids, Gausdal, Norway, 27 August - 1 September 1994 (abstract).

20. "Integration of hydbridization from ab-initio structure calculations, Z. Xiong and N. C. Bacalis, "XV Greek Solid State Conference", edt. A. Zdetsis (Patras, 2000) p. 493 (in Greek).

21. "Analytic atomic wave functions of NMCSCF quality: Applications", Z. Xiong, M.I. Velgakis, and N. C. Bacalis*, Eighth European Workshop on Quantum Systems in Chemistry and Physics : Spetses Island, Greece, August 30 - September 4, 2003 (abstract).

22. "Generalization of Laguerre orbitals toward an accurate, concise and practical analytic atomic wave function", Z. Xiong and N. C. Bacalis*, International Conference of Computational Methods in Sciences and Engineering 2003 (ICCMSE 2003) Kastoria, Greece 12-16 September 2003 (abstract).

23. "Lowest Energy Path of Oxygen near CH: A Combined Configuration Interaction and Tight-Binding Approach", N.C. Bacalis*, A. Metropoulos and D.A. Papaconstantopoulos, International Conference of Computational Methods in Sciences and Enginnering 2004 (ICCMSE 2004), Kavouri, Greece, 19 – 23 November 2004 (abstract).

24. "Accurate and concise atomic CI via generalization of analytic Laguerre type orbitals and examples of ab-initio error estimation for excited states" Z. Xiong, N.C. Bacalis, arXiv:physics/0301062v1 [physics.atom-ph]

25. "Properties of silicon nanocrystals via a transferable tight-binding Hamiltonian, based on ab-initio results", A.D. Zdetsis, N.C. Bacalis*; International Conference of Computational Methods in Sciences and Engineering, Loutraki, Greece, 21-26 October, 2005 (abstract).

26. "Investigation of the reaction between aluminum cluster and methane", E. Alexandrou*, I.D. Petsalakis, H.M. Polatoglou and N.C. Bacalis; CECAM Workshop on "Catalysis from First Principles", Lyon, France, September 11-14 2006 (abstract).

27. "Utilizing the fact that among all trial functions orthogonal to an approximate ground state, $\Phi^0$, the closest, $\Phi^{1+}$, to the exact first excited state,$\psi^1$, has lower energy than the exact: $E[\Phi^{1+}] < E[\psi^1]$", N.C. Bacalis; International Conference on Computational Methods in Science and Engineering (2007). Corfu, Greece, September 25-30, 2007 (abstract).

28. "Remarks on the Hylleraas-Undheim and MacDonald higher roots, and functionals having local minimum at the excited states", N.C. Bacalis*, Z. Xiong and D. Karaoulanis; International Conference on Computational Methods in Science and Engineering (2008); Hersonissos, Crete, Greece, September 25-30, 2008 (invited talk abstract).

29. "Investigation of the reaction between aluminum clusters and methane", E. Alexandrou*, H.M. Polatoglou and N.C. Bacalis; International Conference on Computational Methods in Science and Engineering (2008); Hersonissos, Crete, Greece, September 25-30, 2008 (abstract).

30. "Variational functionals for excited states", N.C. Bacalis, arXiv:0801.3673v1 [quant-ph] (2008)

31. "Remarks On The Standard Hylleraas-Undheim And MacDonald Computation Of Excited States", N.C. Bacalis, arXiv:0809.3826v1 [physics.chem-ph] (2008)

32. "Minimization principle for truncated excited wave functions. Need, Benefits, and Demonstration", Naoum C. Bacalis, International Conference of Computational Methods in Sciences and Engineering, ICCMSE2015, 20-23 March 2015, Athens, Greece (abstract)

33. "Excited state truncated wave functions, lying slightly below the exact: Are they reliable?", Naoum C. Bacalis *, Zhuang Xiong, Jie Zang, Dimitrios Karaoulanis, International Conference of Computational Methods in Sciences and Engineering, ICCMSE2016, 17-20 March 2016, Athens, Greece (abstract)

34. "Excited state truncated wave functions, lying slightly below the exact: Are they reliable?", Naoum C. Bacalis *, Zhuang Xiong, Jie Zang, Dimitrios Karaoulanis, International Conference of Computational Methods in Sciences and Engineering, ICCMSE2016, 17-20 March 2016, Athens, Greece (abstract)

## 1.6 Invited talks

1. "Electron and two-photon momentum density in $TiH_2$ and $ZrH_2$", N.C. Bacalis, Center for Materials Science, Los Alamos National Laboratory, USA, 1988.

2. "One and two - dimensional electron momentum density in vanadium and silver", N.C. Bacalis, Condensed Matter Science seminar, Los Alamos National Laboratory, USA, 1988.

3. "State specific calculations on diatomic molecules", N.C. Bacalis, Condensed Matter and Radiation Sciences Division, Naval Research Laboratory, USA, 1992.

4. "State specific calculations on diatomic molecules", N.C. Bacalis, Condensed Matter and Analytical Sciences Division, Lawrence Livermore National Laboratory, USA, 1992.

5. "Curie temperature in Ni and Fe from APW calculations", N.C. Bacalis, Condensed Matter and Radiation Sciences Division, Naval Research Laboratory, USA, 1995.

6. "Configuration Interaction in diatomic molecules via Simulated Annealing", N.C. Bacalis, Condensed Matter and Radiation Sciences Division, Naval Research Laboratory, USA, 1998.

7. "Curie temperature in Ni and Fe from APW calculations", N.C. Bacalis, Physics Department, University of Athens, Greece, 1998.

8. "Configuration Interaction in diatomic molecules via Simulated Annealing", N.C. Bacalis, Physics Department, University of Athens, Greece, 1998.

9. "Generalization of Laguerre orbitals toward an accurate, concise and practical analytic atomic wave function", N.C. Bacalis, International Conference of Computational Methods In Science and Engineering, Kastoria, Greece, 2003.

10. "Remarks on the Hylleraas-Undheim and MacDonald higher roots, and functionals having local minimum at the excited states", N.C. Bacalis, International Conference on Computational Methods in Science and Engineering 2008; Hersonissos, Crete, Greece, 2008.

11. "Minimization principle for truncated excited wave functions. Need, Benefits, and Demonstration", Naoum C. Bacalis, International Conference of Computational Methods in Sciences and Engineering, ICCMSE2015, 20-23 March 2015, Athens, Greece

12. "Minimization principle for truncated excited wave functions. Need, Benefits, and Demonstration", Naoum C. Bacalis, Research Center for Astronomy and Applied Mathematics of the Academy of Athens, Weekly Seminar in Astronomy and Applied Mathematics, 19 January 2016

13. "Excited state truncated wave functions, lying slightly below the exact: Are they reliable?", Naoum C. Bacalis *, Zhuang Xiong, Jie Zang, Dimitrios Karaoulanis, International Conference of Computational Methods in Sciences and Engineering, ICCMSE2016, 17-20 March 2016, Athens, Greece

14. “Minimization principle for truncated excited wave functions. Need, Benefits, and Demonstration”, Naoum C. Bacalis *, Zhuang Xiong, Jie Zang, Dimitrios Karaoulanis, NCRS Democritos, Weekly Seminar, 19 May 2016