NEKTARIOS N. LATHIOTAKIS

PUBLICATIONS – OCTOBER 2020

A. Ph.D. THESIS

1. "Tight-Binding Molecular Dynamics study of transition metal clusters and the chemisorption of Si and Ni adatoms on the Si(110) surface", Physics Department, University of Crete, (1997).

B. PAPERS IN REFEREED JOURNALS

1. "The applicability of scaling laws in Tight Binding Molecular Dynamics", N. Lathiotakis and A. N. Andriotis, Solid State Comm. 87, 871 (1993).

2. "Tight-Binding Molecular Dynamics Study of transition metal clusters", M. Menon, J. Connolly, N. Lathiotakis and A. Andriotis, Phys. Rev. B 50, 8903 (1994).

3. "Structure and Stability of Ni Clusters: A Tight-Binding Molecular Dynamics Study", N. N. Lathiotakis, A. N. Andriotis, M. Menon and J. Connolly, Europhys. Lett. 29, 135 (1995).

4. "Tight binding molecular dynamics study of Ni clusters", N. N. Lathiotakis, A. N. Andriotis, M. Menon, J Connolly, J. Chem. Phys. 104, 992 (1996).

5. "Magnetic properties of Ni and Fe clusters: a tight binding molecular dynamics study", A. N. Andriotis, N. N. Lathiotakis, M. Menon, Chem. Phys. Lett. 260, 15 (1996).

6. "Magnetic properties of Clusters of Transition Metal Atoms", A. N. Andriotis, N. N. Lathiotakis, M. Menon, Europhys. Lett. 36, 37 (1996).

7. "The reconstruction of the Si(110) surface and its interaction with Si adatoms", M. Menon, N. N. Lathiotakis, A.N. Andriotis, Phys. Rev. B 56, 1412 (1997).

8. "Periods and Damping of the Oscillatory Exchange Coupling across $Cu_{(1-x)}Ni_x$ Alloy Spacer", N. N. Lathiotakis, B. L. Györffy, J. Staunton, B. Ujfalussy, J. Mag. Mag. Matt.

185, 293 (1998).

9. “The Fermi Surface of Random Metallic Alloys and the Oscillatory Magnetic Coupling across Alloy Spacers”, N. N. Lathiotakis, B. L. Györffy, J. Staunton, J. Phys.: Condens. Matter 10, 10357 (1998).

10. “Asymptotic behavior of the Oscillatory Exchange Coupling across Alloy Spacers: a first principles approach”, B. Ujfalussy, N. N. Lathiotakis, B. L. Györffy, J. B. Staunton, Phil. Mag. B 78, 577 (1998).

11. “The dilemma of the Rigid Band Model arising from measurements of the Oscillatory Exchange Coupling across $Cr_{(1-x)}Mo_x$ alloy spacers”, N. N. Lathiotakis, B. L. Györffy, B. Ginatempo, E. Bruno, J. Mag. Mag. Matt. 198, 445 (1999).

12. “Oscillatory Exchange Coupling across $Cr_{(1-x)}V_x$ Alloy spacers”, N. N. Lathiotakis, B. L. Györffy, B. Ginatempo, E. Bruno, S. S. P. Parkin, Phys. Rev. Lett. 83, 215 (1999).

13. “First Principles Asymptotics for the Oscillatory Exchange Coupling in Co/Cu/Co of (100), (110) and (111) orientations”, N. N. Lathiotakis, B. L. Györffy and B. Ujfalussy, Phys. Rev. B 61, 6854 (2000).

14. “Oscillatory Exchange Coupling across $Cu_{(1-x)}Ni_x$ spacers: A first principles calculation of the amplitudes and phases using asymptotic analysis”, N. N. Lathiotakis, B. L. Györffy, E. Bruno, B. Ginatempo, Phys. Rev. B 62, 9005 (2000).

15. “Density functional theory for superconductors”, N. N. Lathiotakis, M. A. L. Marques, M. Lüders, L. Fast, E. K. U. Gross, Int. J. Quantum Chem. 99, 790 (2004).

16. “Ab-initio theory of superconductivity. I Density functional formalism and approximate functionals”, M. Lüders, M. A. L. Marques, N. N. Lathiotakis, A. Floris, G. Profeta, L. Fast, A. Continenza, S. Massidda, E. K. U. Gross, Phys. Rev. B 72, 024545 (2005).

17. “Ab-initio theory of superconductivity. II Application to elemental metals”, M. A. L.

Marques, M. Lüders, N. N. Lathiotakis, G. Profeta, A. Floris, L. Fast, A. Continenza, E. K. U. Gross, S. Massidda, Phys. Rev. B 72, 024546 (2005).

18. "Ab-initio computation of superconducting properties of elemental superconductors and MgB_2", A. Continenza, G. Profeta, A. Floris, C. Franchini, S. Massidda, N. N. Lathiotakis, M. A. L. Marques, M. Lüders and E. K. U. Gross, J. Supercond. 18, 649 (2005).

19. "Superconducting properties of MgB_2 from first principles", A. Floris, G. Profeta, N. N. Lathiotakis, M. Lüders, M. A. L. Marques, C. Franchini, E. K. U. Gross, A. Continenza, S. Massidda, Phys. Rev. Lett. 94, 037004 (2005).

20. "Open shells in reduced-density-matrix-functional theory", N. N. Lathiotakis, N. Helbig, and E. K. U. Gross, Phys. Rev. A 72, 030501(R) (2005).

21. "Superconductivity in Lithium, Potassium, and Aluminum under Extreme Pressure: A First-Principles Study", G. Profeta, C. Franchini, N. N. Lathiotakis, A. Floris, M. A. L. Marques, M. Luders, S. Massidda, E. K. U. Gross, and A. Continenza, Phys. Rev. Lett. 96, 047003 (2006).

22. "Ab initio prediction of pressure-induced superconductivity in potassium", A. Sanna, C. Franchini, A. Floris, G. Profeta, N. N. Lathiotakis, M. Luders, M.A.L. Marques, E. K. U. Gross, A. Continenza, and S. Massidda, Phys. Rev. B 73, 144512 (2006).

23. "Discontinuity of the chemical potential in reduced density matrix functional theory", N. Helbig, N. N. Lathiotakis, M. Albrecht, E. K. U. Gross, Europhys. Lett. 77, 67003 (2007).

24. "Superconducting properties of MgB_2 from first principles", A. Floris, A. Sanna, M. Lüders, G. Profeta, N. N. Lathiotakis, M. A. L. Marques, C. Franchini, E. K. U. Gross, A. Continenza, and S. Massidda, Physica C 453, 45 (2007).

25. "Performance of one-body reduced density matrix functionals for the homogeneous electron gas", N. N. Lathiotakis, N. Helbig, and E. K. U. Gross, Phys. Rev. B 75, 195120

(2007).

26. “Empirical functionals for reduced-density-matrix-functional theory”, M. A. L. Marques and N. N. Lathiotakis, Phys. Rev. A 77, 032509 (2008).

27. Benchmark calculations for reduced density-matrix functional theory”, N. N. Lathiotakis, and M. A. L. Marques, J. Chem. Phys. 128, 184103 (2008).

28. “Theoretical study on tertiary amine-fluorophore photoinduced electron transfer (PET) systems”, I. D. Petsalakis, N. N. Lathiotakis, and G, Theodorakopoulos, J. Mol. Struct.: THEOCHEM 867, 64-70 (2008).

29. “Reduced Density Matrix Functional for Many-Electron Systems”, S. Sharma, J. K. Dewhurst, N. N. Lathiotakis, and E. K. U. Gross, Phys. Rev. B, 78, 201103(R) (2008).

30. “Codoping: A possible pathway for inducing ferromagnetism in ZnO”, N. N. Lathiotakis, A. N. Andriotis, and M. Menon, Phys. Rev. B 78, 193311 (2008).

31. “Tailoring the induced magnetism in Carbon-based and non-traditional inorganic nanomaterials”, A. N. Andriotis, R. M. Sheetz, N. N. Lathiotakis, M. Menon, , Int. J. of Nanotechnology, 6, 164 (2009).

32. “Discontinuity of the chemical potential in RDMFT for open-shell systems”, N. Helbig, N.N. Lathiotakis, E.K.U. Gross, , Phys. Rev A 79, 022504 (2009) .

33. “A functional of the one-body-reduced density matrix derived from the homogeneous electron gas: Performance for finite systems”, N. N. Lathiotakis, N. Helbig, A. Zacarias, E.K.U. Gross, J. Chem. Phys. 130, 064109 (2009).

34. “Density-matrix-power functional: Performance for finite systems and the homogeneous electron gas”, N. N. Lathiotakis, S. Sharma, J. K. Dewhurst, F. G Eich, M. A. L. Marques, and E. K. U. Gross, , Phys. Rev. A 79, 040501(R) (2009).

35. “Optical and magnetic properties of boron fullerenes”, S. Botti, A. Castro, N.N.

Lathiotakis, X. Andrade, M.A.L. Marques, Phys. Chem. Chem. Phys. 11, 4523 (2009).

36. "Emitting and charge transfer electronic states of tertiary amine-fluorophore sensor systems", I. D. Petsalakis, I. S. K. Kerkines, N. N. Lathiotakis, and G. Theodorakopoulos, Chem. Phys. Lett. 474, 278 (2009).

37. "Discontinuities of the chemical potential in Reduced Density Matrix Functional Theory", N. N. Lathiotakis, S. Sharma, N. Helbig, J. K. Dewhurst, M. A. L. Marques, F. G. Eich, T. Baldsiefen, A. Zacarias, and E. K. U. Gross, Zeitschrift für Physikalische Chemie, 224, 467 (2010).

38. "Size consistency of explicit functionals of the natural orbitals in reduced density matrix functional theory", N. N. Lathiotakis, N. I. Gidopoulos, N. Helbig, J. Chem. Phys. 132, 084105 (2010).

39. "Fractional spin in reduced density-matrix functional theory", N. Helbig, G. Theodorakopoulos, and N. N. Lathiotakis, J. Chem. Phys. 135, 054109 (2011).

40. "Ionization potentials and electron affinities from reduced-density-matrix functional theory", E. N. Zarkadoula, S. Sharma, J. K. Dewhurst, E. K. U. Gross, and N. N. Lathiotakis, Phys. Rev A 85, 032504 (2012).

41. "Nonanalyticity of the optimized effective potential with finite basis sets", N. I. Gidopoulos, and N. N. Lathiotakis, Phys. Rev. A 85, 052508 (2012).

42. "Constraining density functional approximations to yield self-interaction free potentials", N. I. Gidopoulos, and N. N. Lathiotakis, J. Chem. Phys. 136, 224109 (2012).

43. "Correlation measures as benchmarks in reduced density matrix functional theory", N. N. Lathiotakis, 113, 762 (2013).

44. "Reply to "Comment on 'Nonanalyticity of the optimized effective potential with finite basis sets' " ", N. I. Gidopoulos, N. N. Lathiotakis, Phys. Rev. A 88, 046502 (2013).

45. “In-plane force fields and elastic properties of graphene”, G. Kalosakas, N. N. Lathiotakis, C. Galiotis, K. Papagelis, J. Appl. Phys. 113, 134307 (2013).

46. “Theoretical study on the electronic structure of triphenyl sulfonium salts: Electronic excitation and electron transfer processes”, Chem. Phys. Lett. 601, 63 (2014).

47. “Local reduced-density-matrix-functional theory: Incorporating static correlation effects in Kohn-Sham equations”, N. N. Lathiotakis, N. Helbig, A. Rubio, N. I. Gidopoulos, Phys. Rev. A 90, 032511 (2014).

48. “Quasi-particle energy spectra in local reduced density matrix functional theory”, N. N. Lathiotakis, N. Helbig, A. Rubio, N. I. Gidopoulos, J. Chem. Phys. 141, 164120 (2014).

49. “Graphene allotropes under extreme uniaxial strain: an ab initio theoretical study”, Z. G. Fthenakis, N. N. Lathiotakis, Phys. Chem. Chem. Phys. 17, 16418 (2015).

50. “Constrained Local Potentials for Self-Interaction Correction”, N. I. Gidopoulos, N. N. Lathiotakis, Adv. Atom. Mol. Opt. Phys. 64, 129 (2015).

51. “Generalized Pauli constraints in reduced density matrix functional theory”, I. Theophilou, N. N. Lathiotakis, M.A.L. Marques, N. Helbig, J. Chem. Phys. 142, 154108 (2015).

52. “Orbitals from local RDMFT: Are they Kohn-Sham or natural orbitals?”, I. Theophilou, N. N. Lathiotakis, N. I. Gidopoulos, A. Rubio, N. Helbig, J. Chem. Phys. 143, 054106 (2015).

53. “Doping induced metal-insulator phase transition in NiO-a reduced density matrix functional theory perspective”, Y. Shinohara, S. Sharma, J. K. Dewhurst, S. Shallcross, N. N. Lathiotakis, E. K. U. Gross, New J. Phys. 17, 093038 (2015).

54. “Spectrum for Nonmagnetic Mott Insulators from Power Functional within Reduced Density Matrix Functional Theory”, Y. Shinohara, S. Sharma, S. Shallcross, N. N. Lathiotakis, E. K. U. Gross, J. Chem. Theory Comput. 11, 4895 (2015).

55. “Tailoring the spacer type and length in push-pull chromophores. Insights from a systematic theoretical study”, I. S. K. Kerkines, N. N. Lathiotakis, G. Theodorakopoulos, I. D. Petsalakis, Chem. Phys. Lett. 653, 178 (2016).

56. “Conditions for Describing Triplet States in Reduced Density Matrix Functional Theory”, I. Theophilou, N. N. Lathiotakis, N. Helbig, J. Chem. Theory Comput. 12, 2668 (2016).

57. “Short-range ordering effects on the electronic Bloch spectral function of real materials in the nonlocal coherent-potential approximation”, A. Marmodoro, A. Ernst, S. Ostanin, L. Sandratskii, P. E. Trevisanutto, N. N. Lathiotakis, and J. B. Staunton, Phys. Rev. B 94, 224205 (2016).

58. “Electron transfer through organic molecular wires: A theoretical study”, N. N. Lathiotakis, G. Theodorakopoulos, I. D. Petsalakis, Chem. Phys. Lett. 667, 45 (2017).

59. “Structural deformations of two-dimensional planar structures under uniaxial strain: The case of graphene”, Z. G. Fthenakis, N. N. Lathiotakis, J. Phys. Cond. Matt. 29, 175401 (2017).

60. “Relating correlation measures: The importance of the energy gap”, C. L. Benavides-Riveros, N. N. Lathiotakis, C. Schilling, M. A. L. Marques, Phys. Rev. A 95, 032507 (2017).

61. “Towards a formal definition of static and dynamic electronic correlations”, C. L. Benavides-Riveros, N. N. Lathiotakis, M. A. L. Marques, Phys. Chem. Chem. Phys. 19, 12655 (2017).

62. “Structural prediction of two-dimensional materials under strain”, P. Borlido, C. Steigemann, N. N. Lathiotakis, M.A.L. Marques and S. Botti, 2D Mater. 4, 045009 (2017).

63. “Atomistic potential for graphene and other sp^2 carbon systems”, Z. G. Fthenakis, G. Kalosakas, G. D. Chatzidakis, C. Galiotis, K. Papagelis, and N. N. Lathiotakis, Phys. Chem. Chem. Phys. 19, 30925 (2017).

64. “Theoretical study on perylene derivatives as fluorescent sensors for amines”, N. N. Lathiotakis, I. S. K. Kerkines, G. Theodorakopoulos, I. D. Petsalakis, Chem. Phys. Lett. 691, 388 (2018).

65. “A torsional potential for graphene derived from fitting to DFT results” G. D. Chatzidakis, G. Kalosakas, Z. G. Fthenakis, and N. N. Lathiotakis, Eur. Phys. J. B, 91, 11 (2018).

66. “Structure of the first order reduced density matrix in three electron systems: A generalized Pauli constraints assisted study”, I. Theophilou, N. N. Lathiotakis, N. Helbig, J. Chem. Phys. 148, 114108 (2018).

67. “Performance of the constrained minimization of the total energy in density functional approximations: the electron repulsion density and potential”, T. Pitts, N. I. Gidopoulos, N. N. Lathiotakis, Eur. Phys. J. B 91, 130 (2018).

68. “Interfacing tetrapyridyl-C-60 with porphyrin dimers via -conjugated bridges: artificial photosynthetic systems with ultrafast charge separation”, C. Stangel, F. Plass, A. Charisiadis, E. Giannoudis, G. Charalambidis, K. Karikis, G. Rotas, G. E. Zervaki, N. N. Lathiotakis, N. Tagmatarchis, A. Kahnt, A. G. Koutsolelos, Phys. Chem. Chem. Phys. 20, 21269 (2018).
69. “Epitaxial highly ordered Sb:SnO2 nanowires grown by the vapor liquid solid mechanism on m-, r-and a-Al2O3”, M. Zervos, N. N. Lathiotakis, N. Kelaidis, A. Othonos, E. Tanasa, E. Vasile, Nanoscale Advances 1, 1980 (2019).
70. “Defect processes in F and Cl doped anatase TiO2”, P-P. Filippatos, N. Kelaidis, M. Vasilopoulou, D. Davazoglou, N. N. Lathiotakis, A. Chroneos, Sci. Rep. 9, 19970 (2019).
71. “Density-inversion method for the Kohn-Sham potential: role of the screening density”, T. J. Callow, N. N. Lathiotakis, and N. I. Gidopoulos, J. Chem. Phys. 152, 164114 (2020).
72. “Improving the exchange and correlation potential in density functional approximations through constraints”, T. Callow, B. J. Pearce, T. Pitts, N. N. Lathiotakis, M. J. Hodgson and N. Gidopoulos, Faraday Discuss., doi:10.1039/D0FD00069H, in press, (2020).
73. “Electronic properties of the $Sn_{1-x}Pb_xO$ alloy and band alignment of the SnO/PbO system: a DFT study”, N. Kelaidis, S. Bousiadi, M. Zervos, A. Chroneos, and N. N. Lathiotakis, Sci. Rep. 10, 16828 (2020).

C. PAPERS IN PROCEEDINGS OF INTERNATIONAL CONFERENCES

1. “Study of Magnetic Clusters Using A Tight Binding Molecular Dynamics Approach”, A. N. Andriotis, N. N. Lathiotakis, M. Menon, Proc.1st International Alloy Conference, Athens 1996, Properties of complex inorganic solids, ed. A. Gonis, A. Meike, P.E.A. Turchi, Plenum Press, 1997, pp. 261-266.

2. “The Fermi surfaces of Metallic Alloys and the Oscillatory Magnetic Coupling between Magnetic Layers separated by such Alloy Spacers”, B. L. Györffy, N. N. Lathiotakis, Properties of complex inorganic solids 2, ed. A. Meike, A. Gonis, P.E.A. Turchi, K. Rajan, Kluwer Academic / Plenum Publishers, 2000, pp. 365-379.

3. “Discontinuities of the Chemical Potential in Reduced Density Matrix Functional Theory”, N. N. Lathiotakis, S. Sharma, N. Helbig, J. K. Dewhurst, M. A. L. Marques, F. G. Eich, T. Baldsiefen, A. Zacarias, E. K. U. Gross, Modern and Universal First Principles

Methods for Many-Electron Systems in Chemistry and Physics, ed. F. M. Dolg, Series Progress in Physical Chemistry, Vol. 3, Oldenburg Verlag, Münhen 2010, p. 179.

D. OTHER PUBLICATIONS

1. Density functional theory for superconductors, M. A. L. Marques, A. Floris, G. Profeta, N. N. Lathiotakis, C. Franchini, A. Sanna, A. Continenza, S. Massidda, E. K. U. Gross, Scientific Highlight of the month, Ψ_k-Newsletter, August 2006: http://www.psi-k.org/newsletters/News_76/Highlight_76.pdf

2. Parallel Implementation of the Reduced Density Matrix Functional Theory for the Development of New Functionals, HPC-Europa 2, Science and Supercomputing in Europe, research highlights 2009, CINECA, Bologna, Italy, ISBN 978-88-86037-23-5.