

List of publications

- [1. C. A. Nicolaides, G. Theodorakopoulos and I. D. Petsalakis, Theory of Chemical Reactions of vibronically excited H₂. Prediction of a strongly bound H₄ excited state, J. Chem. Phys. 80, 1705 \(1984\).](#)
- [2. G. Theodorakopoulos, I. D. Petsalakis, R. J. Buenker and S. D. Peyerimhoff, MRD-CI calculations on the bending potentials of H₂O in the ground and in excited states, Chem. Phys. Lett. 105, 253 \(1984\).](#)
- [3. C.A.Nicolaides, I.D.Petsalakis and G.Theodorakopoulos, Theory of chemical reactions of vibronically excited H₂\(B₁Σ⁺\) III. Formation of bound excited states of the \(H₂\)₂, \(H₂\)₃ and \(H₂\)₅ clusters, J. Chem. Phys. 81,748\(1984\).](#)
- [4. I.D.Petsalakis, G.Theodorakopoulos, C.A.Nicolaides, R.J.Buenker and S.D.Peyerimhoff, Nonorthonormal CI for molecular excited states. I. The sudden polarization effect in 90o twisted ethylene, J. Chem. Phys. 81,3161\(1984\).](#)
- [5. G.Theodorakopoulos, I.D.Petsalakis, I.G.Csizmadia and M.A.Robb, Theoretical and experimental ionization potentials of \(CH₃\)₂S and \(CH₃\)₂SO. The effect of substituents R on the sulphur ESCA shifts in the series R₂S, R₂SO, R₂S, J. Molec. Struct. 110,381 \(1984\)](#)
- [6. I.D.Petsalakis, G.Theodorakopoulos, C.A.Nicolaides and R. J. Buenker, Nonorthonormal CI for molecular excited states. II. The zwitterionic states of terminally twisted butadiene. J. Chem. Phys. 81,5952\(1984\).](#)
- [7. G.Theodorakopoulos, I.D.Petsalakis, C.A.Nicolaides and R.J.Buenker, The X 1A₁— A 1B₁ transition moment of H₂O using State-Specific Configuration Interaction wavefunctions. J. Chem. Phys. 82,912\(1985\).](#)
- [8. G.Theodorakopoulos, I.D.Petsalakis and R.J.Buenker, MRD-CI calculations on the asymmetric stretch potentials of H₂O in the ground and the first seven singlet excited states, Chem. Phys. 96,217\(1985\)](#)
- [9. G.Theodorakopoulos, I.D.Petsalakis, C.A.Nicolaides and R.J.Buenker, Configuration interaction study of the oscillator strengths for the B 1A₁— X 1A₁ and D 1A₁— X 1A₁ transitions of the water molecule, Chem. Phys. 100,331\(1985\).](#)
- [10. G.Theodorakopoulos, I.D.Petsalakis and C.A.Nicolaides, A method for the calculation of transition moments between electronic states of molecules using a different one-electron basis set for each state, Inter. J. Quantum Chem. 29,399\(1986\).](#)
- [11. G.Theodorakopoulos, I.D.Petsalakis and C.A.Nicolaides. Potential energy hypersurfaces of H₄ in the ground and the first two singlet excited electronic states. J. Molec. Struct. 149,23\(1987\).](#)
- [12. G.Theodorakopoulos,I.D.Petsalakis, C.A.Nicolaides and R.J.Buenker, Nonorthonormal basis calculations of the transition moment for the Phillips system \(A 1Π_u— X 1Σ_g⁺\) in C₂. Theoretical lifetime of the A 1Π_u state. Chem. Phys. 112,319\(1987\).](#)

- [13. G.Theodorakopoulos, I.D.Petsalakis and R.J.Buenker. states of H₂O along a linear dissociation path leading to OH+H. Chem. Phys. Let. 138,71\(1987\).](#)
- [14. G.Theodorakopoulos, I.D.Petsalakis,C.A.Nicolaides and R.J.Buenker, Theoretical dipole transition moments for the transitions to the ground state X \$2\Sigma^+\$ from the A \$2\Sigma^+\$, B \$2\Pi\$, C \$2\Sigma^+\$, D \$2\Sigma^+\$ and E \$2\Pi\$ states and the B \$2\Pi\$ — A \$2\Sigma^+\$ system in HeH, J. Phys. B: At. Mol. Phys. 20,2339\(1987\).](#)
- [15. G.Theodorakopoulos, I.D.Petsalakis and R.J.Buenker, Theoretical investigation of the excited states of NeH: Calculations of dipole transition moments and radial coupling matrix elements, J. Phys. B: At. Mol. Phys. 20,5335\(1987\).](#)
- [16. I.D.Petsalakis, G.Theodorakopoulos, C.A.Nicolaides and R.J.Buenker, Theoretical dipole transition moments for transitions between bound electronic states and non-adiabatic coupling matrix elements between \$2\Sigma^+\$ states of HeH, J. Phys. B: At. Mol. Phys. 20,5959\(1987\).](#)
- [17. I.D.Petsalakis, G.Theodorakopoulos, J.S.Wright and I.P.Hamilton,The Rydberg states of FH₂, J. Chem. Phys. 88,7633\(1988\).](#)
- [18. G.Theodorakopoulos, I.D.Petsalakis, and R.J.Buenker. Non-adiabatic interactions between the C \$2\Sigma^+\$ and D \$2\Sigma^+\$ electronic states of HeH, Chem. Phys. Let. 148,285\(1988\).](#)
- [19. G.Theodorakopoulos and I.D.Petsalakis, Ab initio calculations on the ground and excited electronic states of KrH.Chem.Phys. Let. 149,196\(1988\).](#)
- [20. I.D.Petsalakis, G.Theodorakopoulos and R.J.Buenker, Radiative dissociation and predissociation in HeH and NeH: A theoretical treatment using square-integrable functions. Phys. Rev. A 38,4004\(1988\).](#)
- [21. I.D.Petsalakis, G.Theodorakopoulos, J.S.Wright and I.P.Hamilton, Theoretical investigation involving electronic and vibrational calculations of the \$2A_1\(3p\)\$ — \$1\ 2B_2\(3p\)\$ and the \$3\ 2A_1\(4s\)\$ — \$1\ 2B_2\(3p\)\$ transitions in FH₂ and FD₂. J.Chem. Phys. 89,6841 \(1988\).](#)
- [22. I.D.Petsalakis, G.Theodorakopoulos and J.S.Wright, Theoretical calculations on electronic transitions for H₃, including Rydberg and transition state spectra. J. Chem. Phys. 89, 6850 \(1988\).](#)
- [23. P.Karafiloglou, G.Theodorakopoulos and I.D.Petsalakis,Valence bond analysis of molecular orbital wavefunctions. The ionicity of the B \$1\Sigma^+\$ state of H₂. J. Molec. Stuct. THEOCHEM 180,31 \(1988\).](#)
- [24. I.D.Petsalakis and G.Theodorakopoulos, Theoretical calculations on radiative and nonradiative processes of quartets states of HeH, Chem. Phys. 130,211 \(1989\).](#)
- [25. I. D. Petsalakis, A. Metropoulos, G. Theodorakopoulos, and C. A. Nicolaides , An estimate of the lifetime of excited tetrahydrogen, Chem. Phys. Lett. 158,229 \(1989\).](#)
- [26. I. D. Petsalakis, G. Theodorakopoulos, and V. Barclay, Theoretical calculations on the ground electronic state of NeHe⁺, Chem. Phys. Letters 160,189\(1989\).](#)

- [27. G. Theodorakopoulos, I.D. Petsalakis, R.J. Buenker and M.Honigmann, Theoretical calculations on the radiative lifetime of the A \$2\Delta\$ state of CH, Chem. Phys. 137,137 \(1989\).](#)
- [28. I. D. Petsalakis, T. Mercouris, G. Theodorakopoulos and C. A. Nicolaidis, Predissociation resonances from a complex eigenvalue Schroedinger equation. J. Phys. B.23, L89\(1990\)](#)
- [29. I. D. Petsalakis, G. Theodorakopoulos and R. J. Buenker, Theoretical treatment of predissociation in the A \$2\Sigma^+\$, B \$2\Pi\$ and C \$2\Sigma^+\$ states of HeH. J. Chem. Phys.92 4920 \(1990\)](#)
- [30. I.D. Petsalakis, G. Theodorakopoulos, J. S. Wright and I. P. Hamilton, Potential energy surface for large-amplitude motion and vibrational spacing for FH \$2^+\$, J.Chem.Phys.92, 2440 \(1990\).](#)
- [31. G.Theodorakopoulos, I.D.Petsalakis and R.J.Buenker, Theoretical calculations of the Rydberg spectra of ArH, Molec.Phys. 71, 1055 \(1990\)](#)
- [32. I.D. Petsalakis, Th. Mercouris, G. Theodorakopoulos and C. A. Nicolaidis, Distributed Complex Gaussian basis sets: A useful function space for the solution of predissociation problems by the isotope effect of NeH,NeD.J. Chem.Phys. 93,6642\(1990\).](#)
- [33. G. Theodorakopoulos and I.D.Petsalakis, Theoretical Study of CH \$2^+\$ J.Mol.Struct. \(Theochem\) 230 , 205 \(1991\)](#)
- [34. I.D.Petsalakis, Electronic structure and lifetime of an excimer state of HeF, J. Chem. Phys. 94, 2906 \(1991\)](#)
- [35. G. Theodorakopoulos and I.D.Petsalakis, Asymmetric dissociation and bending potentials of H \$2\$ S in the ground and excited electronic states, Chem.Phys.Lett. 178, 475 \(1991\).](#)
- [36. I. D. Petsalakis, Th. Mercouris, G. Theodorakopoulos and C.A. Nicolaidis, Theory and ab-initio calculations of partial widths and interchannel coupling in predissociating diatomic states. Application to HeF. Chem.Phys.Lett. 182, 561 \(1991\)](#)
- [37. I. D. Petsalakis, G. Theodorakopoulos, C. A. Nicolaidis and R.J.Buenker, Nearly-diabatic states by maximization of the non-orthonormal overlap between model-diabatic and MRD-CI wavefunctions, Chem.Phys.Lett. 185, 359 \(1991\)](#)
- [38. I.D. Petsalakis, G. Theodorakopoulos and S.Consta, Theoretical calculations on the electronic states XeH, Mol.Phys. 75, 805 \(1992\).](#)
- [39. I. D. Petsalakis, G. Theodorakopoulos and C.A.Nicolaidis, Adiabatic and Quasi-diabatic \$2\Sigma^+\$ states of BeH, J. Chem.Phys. 97, 7623 \(1992\).](#)
- [40. I. D. Petsalakis and G. Theodorakopoulos, Theoretical Calculations on Rydberg states of H \$2\$ S, Chem.Phys.Lett .200, 387 \(1992\).](#)
- [41. I. D. Petsalakis and G. Theodorakopoulos, Theoretical lifetimes of Rydberg states of ArH and ArD, J.Phys.B25, 5353 \(1992\).](#)

- [42. Th.Mercouris, I. D. Petsalakis and C.A.Nicolaidis, Time-dependent laser-induced molecular formation from repulsive surfaces, Chem. Phys. Let. 208, 197 \(1993\)](#)
- [43. G. Theodorakopoulos, I. D. Petsalakis and C. A. Nicolaidis, Diabatic potentials for the 11A" and 21A" states of H2S. Chem. Phys. Lett.207,321\(1993\).](#)
- [44. G. Theodorakopoulos and I. D. Petsalakis, Potential energy curves and radiative lifetimes of Rydberg states of NaHe. J.Phys. B26 4367 \(1993\).](#)
- [45. C.A. Nicolaidis, Th. Mercouris and I.D.Petsalakis, Above and below threshold multiphoton dissociation of volcanic ground states. Application to BeH⁺⁺ , Chem. Phys Let. 212, 685 \(1993\)](#)
- [46. C.A.Nicolaidis, Th. Mercouris, Y.Komninou and I.D.Petsalakis, Many-electron, many-of photon theory nonstationary states, Int. J. of Quant.Chem, 51,529 \(1994\)](#)
- [47. I. D. Petsalakis, G. Theodorakopoulos and C. A. Nicolaidis,Quasi-diabatic states for intramolecular charge transfer.Application to the protonation of NH₃, J. Chem. Phys. 100, 5870 \(1994\).](#)
- [48. G. Theodorakopoulos and I. D. Petsalakis,Rydberg spectra of ArH. Bound-Bound interactions and lifetimes of the Rydberg states. J. Chem.Phys. 101, 194 \(1994\).](#)
- [49. J.-ping Gu, G. Hirsch, R. J. Buenker, I. D. Petsalakis, G. Theodorakopoulos and M.-ba Huang,Electronic states and radiative transitions in LiAr, Chem. Phys. Lett.230, 473 \(1994\).](#)
- [50. Th. Mercouris, I.D.Petsalakis,P.Valtzanos and C.A.Nicolaidis, Time-dependent multiphoton absorption by NO⁺⁺. Above and below threshold dissociation and the effect of the first excited surface, J.Phys. B 27 ,L519 \(1994\)](#)
- [51. I.D.Petsalakis,Th. Mercouris and C.A.Nicolaidis, Computation of time-dependent transition probabilities in excimer molecules induced by femtosecond laser pulses, Chem. Phys. 189, 615 \(1994\).](#)
- [52. I.D. Petsalakis and G. Theodorakopoulos,Ion-pair and Rydberg states of ArH, J.Phys. B 27, 4483 \(1994\).](#)
- [53. I.D. Petsalakis G. Theodorakopoulos and M.S. Child, Ab initio multichannel quantum defects for the 1A1 Rydberg states of H₂O. J.Phys. B 28 ,5179 \(1995\).](#)
- [54. G. Theodorakopoulos, I.D.Petsalakis and M.S.Child, On the construction and use of ab initio quantum defect functions for H₂O. J. Phys B 29,4543 \(1996\)](#)
- [55. Yan Li, I.D.Petsalakis,H.P.Liebermann, G.Hirsch and R.J.Buenker, Ab initio configuration interaction calculations of the predissociation of rovibrational levels of the C 3Πg and d 1Πg 3σ Rydberg states of the oxygen molecule. J.Chem.Phys. 106,1123 \(1997\)](#)
- [56. I.D.Petsalakis ,R.J.Buenker, G.Hirsch and G.Theodoarakopoulos, Predissociation widths and lifetimes of the n=3 2Σ⁺ states of BeH, J.Phys. B, 30,4935 \(1997\)](#)

- [57. I. D. Petsalakis G. Theodorakopoulos, Yan Li, G.Hirsch, R.J.Buenker and M.S. Child, Theoretical study on the Rydberg states of NeH. Ab initio, quantum defect and complex coordinate calculations, J. Chem. Phys. 108,7607 \(1998\)](#)
- [58. G. Theodorakopoulos, I. D. Petsalakis and M.S. Child, An ab initio potential energy surface and spectroscopic constants for the \$X1\Sigma_g^+\$ state of \$\text{NO}_2^+\$, J.Molec. Struct., Theochem 434,177 \(1998\)](#)
- [59. D. Azinovic, Ch. Wunderlich, H. Figger, G. Theodorakopoulos and I.D. Petsalakis, Dynamics on the ground state potential surface of \$\text{H}_3\$ Phys. Rev. A 58, 1115 \(1998\)](#)
- [60. I.D Petsalakis, Theoretical study on electronic states of carbon monofluoride and on the predissociation of the lower lying states, J. Chem. Phys. 110, 10730 \(1999\)](#)
- [61. M. Honigmann, G. Hirsch, R.J. Buenker, I.D. Petsalakis and G. Theodorakopoulos, Complex coordinate calculations on autoionizing states of HeH and \$\text{H}_2\$, Chem. Phys. Let. 465, 305 \(1999\)](#)
- [62. I.D. Petsalakis, D. Papadopoulos, G. Theodorakopoulos and R.J. Buenker, Theoretical calculations on the linewidths of rovibrational levels of the 3d Rydberg states of BeH and BeD. J. Phys. B. 3225, 32, \(1999\)](#)
- [63. G. Theodorakopoulos, I.D. Petsalakis and I.P. Hamilton, Ab Initio calculations on the ground and excited states of BeOH and MgOH, J. Chem. Phys. 10484, 111, \(1999\)](#)
- [64. I.D. Petsalakis and G. Theodorakopoulos, Electronic states of \$\text{CF}^+\$ Chem. Phys. 181, 254 \(2000\)](#)
- [65. I.D. Petsalakis, R.J. Buenker, H.P. Lieberman, A.B. Alekseyev, A.Z. Dendariani and G. Theodorakopoulos, Potential energy curves and dipole transition moments to the ground state of the system \$\text{Ar}^* \(3p54s, 3P, 1P\) + \text{Ne}\$. J. Chem. Phys. 5812, 113 \(2000\)](#)
- [66. I.D. Petsalakis, G. Theodorakopoulos, H.P. Lieberman and R.J. Buenker, Potential energy curves and dipole transition moments for electronic states of ArHe and HeNe. J. Chem. Phys. 115, 6365 \(2001\)](#)
- [67. I.D. Petsalakis, G. Theodorakopoulos and M.S. Child, The Rydberg states of \$\text{NO}_2\$. Vibrational autoionization of the \$n\sigma\$ states. J. Chem. Phys. 115, 10394 \(2001\)](#)
- [68. K. Das, I.D. Petsalakis, H.P. Lieberman and R.J. Buenker, Ab initio spin-orbit configuration interaction calculation for potential curves and radiative lifetimes of the low-lying electronic states of Lead monofluoride. J. Chem. Phys. 116, 608 \(2002\)](#)
- [69. G. Theodorakopoulos, I.D. Petsalakis and M.S. Child, On the construction and use of ab initio quantum defect functions for the Rydberg spectra of molecules. Rus. J. Phys. Chem. 76, S95 \(2002\)](#)
- [70. I.D. Petsalakis, G. Theodorakopoulos and R.J. Buenker, Complex coordinate calculations on predissociating states of diatomic molecules. Russian Journal of Phys. Chem. 76, S1 \(2002\)](#)

- [71. I.D.Petsalakis, G.Theodorakopoulos, H.P.Lieberman and R.J.Buenker , Potential energy curves and dipole transition moments for excited electronic states of XeKr and ArNe. J.Chem.Phys.117 3639 \(2002\)](#)
- [72. G.Theodorakopoulos,I.D.Petsalakis, H.P.Lieberman, R.J.Buenker and J.Kopot, Ab initio calculations on electronic states of CaOH. J.Chem. Phys. 117 4810 \(2002\)](#)
- [73. J.Luque, E.A.Hudson,J.P.Booth and I.D.Petsalakis, Broadband absorption and ab initio results on the CF C2Σ+ - X2Π system.J. Chem. Phys.118,1206 \(2003\)](#)
- [74. I.D.Petsalakis, G.Theodorakopoulos and R.J.Buenker, Theoretical ab initio study of the electronic states of KrH and KrH+..Quantum defect and complex coordinate calculations on the Rydberg states of KrH. J.Chem.Phys. 119 2004 \(2003\)](#)
- [75. I.D.Petsalakis, J.C.Polanyi and G Theodorakopoulos , Theoretical study of the induced attachment of benzene to Si\(111\) 7X7. Surface Science 544 162 \(2003\)](#)
- [76. I.D.Petsalakis, G.Theodorakopoulos, R.W.Gora and S.Roszak, Theoretical ab initio Study on the Electronic states of GaO and Ga2O. TheoChem, Journal of Mol. Struct.672 105 \(2004\)](#)
- [77. K. Rajamma Harikumar, Ioannis D. Petsalakis, John C. Polanyi, and Giannoula Theodorakopoulos, Theoretical study of the halogenation reactions of 1,2- and 1,4-dibromobenzene at Si\(111\)-7×7, Surface Science 572 162 \(2004\)](#)
- [78. I.D.Petsalakis, J.C.Polanyi and G Theodorakopoulos , Theoretical study of the of benzene, toluene and dibromobenzene at a Si\(111\) 7X7 surface, Israel J. of Chemistry, 45 111 \(2005\)](#)
- [79. I. D. Petsalakis and G. Theodorakopoulos, Theoretical study of halogen-substituted benzene on a Si\(111\)7X7 surface, Israel J. of Chemistry, 45 127 \(2005\)](#)
- [80. I. D. Petsalakis and G. Theodorakopoulos, Multireference configuration interaction and quantum defect calculations on the Rydberg states of the BH molecule, Molecular Physics 104 103 \(2006\)](#)
- [81. G. Theodorakopoulos and I.D.Petsalakis, Theoretical study on the low-lying electronic states of InN, Chem. Phys. Let 423 445 \(2006\)](#)
- [82. I.D.Petsalakis, G.Pagona, G. Theodorakopoulos, N.Tagmatarchis, M.Yudasaka and S.Iijima, Unbalanced strain-directed functionalization of carbon nanohorns. A theoretical investigation based on complementary methods, Chem. Phys. Let. 429 194 \(2006\)](#)
- [83. A.Devdariani, E.Tchesnokov, A.Zagrebin, M.G.Lednev, I.D.Petsalakis, G.Theodorakopoulos, H.P.Lieberman and R.J.Buenker, Quasi-molecular radiative transitions produced by thermal and low-temperature collisions Ar\(3p6 1S0-3p54s 3P2\)-He, Chemical Physics 330 101 \(2006\)](#)

- [84. I. D. Petsalakis and G. Theodorakopoulos, Theoretical study of nonadiabatic interactions, radiative lifetimes and predissociation lifetimes of excited states of BH, Molecular Physics 105 333 \(2007\)](#)
- [85. I.D.Petsalakis, N.Tagmatarchis, G.Rotas and G.Theodorakopoulos, Theoretical study on triphenylamine-based sensors of dicarboxylic acids, J. Molecular Structure 807 11 \(2007\)](#)
- [86. D.Emfietzoglou, H.Nikjoo, I.D.Petsalakis and A.Pathak, A consistent dielectric response model for water ice over the whole energy-momentum plane, Nuclear Instruments and methods in Physics Research B 256,141 \(2007\)](#)
- [87. G.Pagona, G.Rotas, I.D.Petsalakis, G.Theodorakopoulos, J.Fan, A.Maigne, M.Yadasaka, S.Iijima and N.Tagmatarchis, Soluable functionalized carbon nanohorns, J. Nanoscience and Nanotechnology, 7, 3468 \(2007\)](#)
- [88. G.Pagona, A.S.D. Sandanayaka, A. Maigne, J. Fan, G.C. Papavassiliou, I.D.Petsalakis, B.R. Steele, M. Yudasaka, S. Iijima, N. Tagmatarchis and O. Ito, Photoinduced electron transfer on aqueous carbon nanohorn-pyrene tetrathiafulvalene architectures, Chem. Eur. J. 13, 7600 \(2007\)](#)
- [89. I.D.Petsalakis, N.Tagmatarchis and G.Theodorakopoulos, Theoretical study of fulleropyrrolidines by density functional and time-dependent density functional theory, J. Phys. Chem. C 111\(38\), 14139 \(2007\)](#)
- [90. D. Tzeli, I.D. Petsalakis and G. Theodorakopoulos, Theoretical investigation on the electronic and geometric structure of GaN₂⁺ and GaN₄⁺, J. Phys. Chem. A 111\(36\), 8892 \(2007\)](#)
- [91. D. Tzeli, I.D. Petsalakis and G. Theodorakopoulos, Theoretical study of adsorption of gallium and gallium nitrides on Si\(111\), Chem. Phys. Lett. 448, 88 \(2007\)](#)
- [92. I.D.Petsalakis, G. Pagona, N.Tagmatarchis and G.Theodorakopoulos, Theoretical study in donor-acceptor carbon nanohorn-based hybrids, Chem. Phys. Lett. 448, 115 \(2007\)](#)
- [93. Lukáš Demovič, Ivan Černušák, Giannoula Theodorakopoulos, Ioanis D. Petsalakis and Miroslav Urban, Improved theoretical calculations of InN in its X₃Σ⁻ ground state and in the first 3Π excited state, Chem. Phys. Lett. 447, 215 \(2007\)](#)
- [94. D.Emfietzoglou, I.Abril, R.Garcia-Molina, I.D.Petsalakis, H.Nikjoo, A.Pathak, Semi-empirical dielectric descriptions of the Bethe surface of the valence bands of condensed water, Nuclear Instruments and methods in Physics Research B 266, 1154 \(2008\)](#)
- [95. L.Šimová, D. Tzeli, M. Urban, I. Černušák, G. Theodorakopoulos, I. D. Petsalakis, Structure and Energetics of InN and GaN Dimers, Chem. Phys. 349,98 \(2008\)](#)

- [96. I.D.Petsalakis ,D.Tzeli and G. Theodorakopoulos, Theoretical study on the electronic states of NaLi, J.Chem.Phys 129,054306 \(2008\)](#)
- [97. D.Tzeli, G.Theodorakopoulos and I.D.Petsalakis, Theoretical study of Gallium Nitride Molecules, GaN₂ and GaN₄. J.Phys.Chem.A 112, 8858 \(2008\)](#)
- [98. I.D.Petsalakis, N.N. Lathiotakis and G.Theodorakopoulos, Theoretical study on tertiary amine-fluorophore photoinduced transfer \(PET\) systems, J.Mol. Struct. \(Theochem.\) 867, 64 \(2008\)](#)
- [99. I.D.Petsalakis and G.Theodorakopoulos, Photoinduced charge transfer in fullerene-donor dyads: A theoretical study. Chem. Phys. Lett. 466, 189 \(2008\)](#)
- [100. D.Emfietzoglou, I.Kyriakou I.Abril, R.Garcia-Molina, I.D.Petsalakis, H.Nikjoo, A.Pathak, Electron inelastic mean free paths in biological matter based on dielectric theory and local-field corrections, Nuclear Instruments and methods in Physics Research B 267, 45 \(2009\)](#)
- [101. D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos. “Theoretical study of adsorption of group IIIA nitrides on Si\(111\)”, J. Phys. Chem. C 113, 5563 \(2009\)](#)
- [102. K. Ghosh, G. Masanta, R. Fröhlich, I. D. Petsalakis and G.Theodorakopoulos “Triphenylamine-based receptors in selective recognition of dicarboxylic acids” J. Phys. Chem. B 113, 7800 \(2009\)](#)
- [103. I.D. Petsalakis, I.S.K. Kerkines, N.N. Lathiotakis and G. Theodorakopoulos “Emitting and electron-transfer electronic states of tertiary amine-fluorophore sensor systems” , Chem. Phys. Lett. 474, 278 \(2009\).](#)
- [104. D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos “Theoretical Study of Adsorption and Diffusion of Group IIIA Metals on Si\(111\)”, J. Phys. Chem. C 113,13924 \(2009\)](#)
- [**105. D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, Theoretical investigation of the ground and low-lying excited states of Gallium and Indium Silicides, GaSi and InSi. J.Chem. Phys. 131, 234301 \(2009\)**](#)
- [106. I. Kerkines, I. D. Petsalakis, G. Theodorakopoulos, and W. Klopper, Low-lying absorption and emission spectra of pyrene, 1,6-dithiapyrene and tetrathiafulvalene: a comparison between ab initio and time-dependent density functional methods, J.Chem.Phys. 131,224315 \(2009\)](#)
- [107. I. D. Petsalakis, G. Theodorakopoulos , A. Grochol, P. Kowalczyk, W. Jastrzebski, Theoretical study of highly excited 1Sigma⁺ and 1P states of NaLi and experimental observation of the interacting 5 1Sigma⁺ and 6 1Sigma⁺ states, Chem. Phys.362, 130 \(2009\)](#)
- [108. D. Irimia, I. D. Petsalakis, G. Theodorakopoulos and M. H.M. Janssen, Coherent oscillatory femtosecond dynamics in multichannel photodynamics of NO₂ studied by spatially masked electron imaging, J. Phys. Chem. A 114, 3157 \(2010\)](#)

- [109. K. Ghosh, T. Sen, R. Fröhlich, I. D. Petsalakis and G. Theodorakopoulos, Trans-pyridyl and naphthyridyl cinnamides as alternatives of urea in complexation of carboxylic acid and formation of water-templated assemblies in the solid state, J. Phys. Chem. B 114, 321 \(2010\)](#)
- [110. I.D.Petsalakis, D.Georgiadou, M.Vasilopoulou, G.Pistolis, D.Dimitrokali, P.Argitis and G.Theodorakopoulos, "Theoretical Investigation on The Effect of Protonation on The Absorption and Emission Spectra of Two Amine-Group-Bearing, Red "Push-Pull" Emitters, 4-Dimethylamino-4'-Nitrostilbene \(DANS\) and 4-\(Dicyanomethylene\)-2-Methyl-6-p-\(Dimethylamino\) Styryl-4H-Pyran \(DCM\), by DFT and TDDFT Calculations", J. Phys. Chem. A 114, 5580 \(2010\)](#)
- [111. I. S. K. Kerkines, I. D. Petsalakis, G. Theodorakopoulos and J. Rebek, Jr, "Excited state intramolecular proton transfer in hydroxy oxime-based chemical sensors" The J. Phys. Chem. A. 115, 834 \(2011\)](#)
- [112. D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, Theoretical investigation of the complexation of crown ethers and crown ethers of fulleropyrrolidine with \(CH₃\)_xNH_{4-x} x = 0 – 4 Phys.Chem.Chem.Phys.13,954 \(2011\)](#)
- [113. I. D. Petsalakis, D. Tzeli, Ioannis S. K. Kerkines and G. Theodorakopoulos, "Theoretical study on the electronic structure and the absorption spectra of complexes of C₆₀ and C₅₉N with \$\pi\$ -extended derivatives of tetrathiafulvalene" Comp. and Theor. Chem.965, 168 \(2011\)](#)
- [114. Ioannis Thanopoulos, Ioannis D. Petsalakis, and Giannoula Theodorakopoulos, Photoinduced charge transfer in heterofullerene-donor hybrids: A theoretical study Chem.Phys.Lett. 506, 248 \(2011\)](#)
- [115. I. D. Petsalakis and G. Theodorakopoulos "Theoretical calculations on the potential energy curves of electronic states of CF. Rydberg states of CF above the lowest ionization limit" Chem.Phys.Lett. 508, 17 \(2011\)](#)
- [116. D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos " Electronic structure and absorption spectra of supramolecular complexes of a fullerene crown ether with a \$\pi\$ -extended TTF derivative" Phys. Chem. Chem. Phys. 13 \(25\): 11965-11975 \(2011\)](#)
- [117. K. Ghosh, S. Adhikari, R. Fröhlich, I. D. Petsalakis, G. Theodorakopoulos " Experimental and theoretical anion binding studies on coumarin linked thiourea and urea molecules \(J. Mol. Structure 1004, 193 \(2011\)](#)
- [118. I.S. K. Kerkines, I. D. Petsalakis, G. Theodorakopoulos and P.Argitis "Fluorescence properties of organic dyes: Quantum chemical studies on the green/blue neutral and protonated DMA-DPH emitters in polymer matrices" Phys. Chem. Chem. Phys. 13, 21273-21281, \(2011\)](#)
- [119. D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, " Computational insight into the electronic structure and absorption spectra of Lithium complexes of N-confused porphyrin" J. Phys. Chem A 115, 11749 \(2011\)](#)

- [120. D.Tzeli, G. Theodorakopoulos, I. D. Petsalakis, Dariush Ajami and Julius Rebek, Jr, "Theoretical study of hydrogen bonding in homodimers and heterodimers of amide, boronic acid and carboxylic acid, free and in encapsulation complexes" J. Amer. Chem.Soc.16977, 133\(42\) \(2011\)](#)
- [121. I.D.Petsalakis and G.Theodorakopoulos, " Molecular orbital assistance in the design of intramolecular and photoinduced electron transfer systems",Chem. Phys.Lett., 525,105-109 \(2012\)](#)
- [122. D.Tzeli, G. Theodorakopoulos, I. D. Petsalakis, Dariush Ajami and Julius Rebek, Jr,"Conformations and fluorescence of encapsulated stilbene" J. Amer. Chem.Soc.134, 4346 \(2012\)](#)
- [123. D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, Dariush Ajami, Wei Jiang and Julius Rebek, Jr " Encapsulated hydrogen-bonded dimers of amide and carboxylic acid" Chem. Phys Let. 548,55 \(2012\)](#)
- [124. D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, " A Theoretical Study of Complexes of Crown Ethers with Substituted Ammonium Cations", ADVANCES IN THE THEORY OF QUANTUM SYSTEMS IN CHEMISTRY AND PHYSICS Book Series: Progress in Theoretical Chemistry and Physics: 22 , 599-610 \(2012\) DOI: 10.1007/978-94-007-2076-3 31](#)
- [125. D.Tzeli, G. Theodorakopoulos, I. D. Petsalakis, Dariush Ajami and Julius Rebek, Jr," Theoretical Study of Free and Encapsulated Carboxylic Acid and Amide Dimers" Int.Journal of Quantum Chem.113, 734 \(2013\)](#)
- [126. D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, " Compression in encapsulated carboxylic acid homodimers" Chem. Phys Let. 573, 48 \(2013\)](#)
- [127. Kumares Ghosh, Sk. Sarfaraj Ali, Avik Ranjan Sarkar, Asmita Samadder, Anisur Rahman , Khuda-Bukhsh, Ioannis D. Petsalakis and Giannoula Theodorakopoulos, "Pyridinium-based tripodal chemosensor invisible sensing of AMP in water by indicator displacement assay \(IDA\)", \(Organic and Biomolecular Chemistry, 11, 5666 \(2013\)](#)
- [128. D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos "Theoretical study on the electronic structure, formation and absorption spectra of Lithium, Sodium and Potassium Complexes of N-confused Tetraphenylporphyrin", Com. Theor. Chem. , 1020, 38-50 \(2013\)](#)
- [129. M. G. Sarwar, D. Ajami, G. Theodorakopoulos, I. D. Petsalakis, and J. Rebek, Jr, " Amplified Halogen Bonding in a Small Space" , J. Amer.Chem.Soc. 135,13672 \(2013\)](#)
- [130. I. D. Petsalakis and G. Theodorakopoulos, Boronic Acid sensors for saccharides: A theoretical study , Chem. Phys.Let. 586,111 \(2013\)](#)

- [131. D. Ajami, G. Theodorakopoulos, I. D. Petsalakis, and J. Rebek, Jr." Social Isomers of Picolines in a Small Space" , Chem. Eur. J. 19, 17092 \(2013\)](#)
- [132. D. G. Georgiadou, M. Vasilopoulou¹, L. C. Palilis³, I. D. Petsalakis⁴, G. Theodorakopoulos⁴, V. Constantoudis¹, S. Kennou⁵, A. Karantonis², D. Dimotikali² and P. Argitis , "All-organic solution processed sulfonium salts acting as electron injection layer for PLEDs " ACS Applied Materials & Interfaces 5, 12346 \(2013\)](#)
- [133. N. Karakostas, I. M. Mavridis¹, K. Seintis², M. Fakis², E. N. Koini, I. D. Petsalakis and G.Pistolis. "Highly efficient and unidirectional energy transfer within a tightly self-assembled host–guest multichromophoric array ChemCom, 50, 1362 \(2014\)](#)
- [134. Ioannis D. Petsalakis, Giannoula Theodorakopoulos, Nektarios N. Lathiotakis, Dimitra G. Georgiadou, Maria Vasilopoulou, Panagiotis Argitis "Theoretical study on the electronic structure of Triphenyl sulfonium Salts: Electronic excitation and charge transfer processes", Chem. Phys. Let. 601,63-68 \(2014\)](#)
- [135. I. D. Petsalakis and G. Theodorakopoulos, "Theoretical study on a corrole-azafullerene dyad: Electronic structure, spectra and photoinduced electron transfer", Chem. Phys. Let. 610-611, 50-55 \(2014\)](#)
- [136. Kumares Ghosh, Debasis Kar, Atanu Panja, Ioannis D. Petsalakis and Theodorakopoulos, "Benzimidazolium-based new simple ratiometric fluorescent Giannoula sensor for selective detection of dihydrogenphosphate" Supramolecular Chemistry , 26, 856, \(2014\)](#)
- [137. D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, Dariush Ajami, and Julius Rebek, Jr, "The Role of the Host-Guest Interactions in the Relative Stability of Compressed Encapsulated Homodimers and Heterodimers of Amides and Carboxylic Acids", Theor.Chem.Act. 133, 1503 \(2014\)](#)
- [138. B.Pappas, I.D.Petsalakis, G.Theodorakopoulos and J.Whitten "CI and DFT Studies of the Adsorption of the Nerve Agent Sarin on Surfaces" J. Phys. Chem. C, 23042 \(2014\).](#)
- [139. Paweł Kozieliwicz, Petros G. Tsoungas, Demeter Tzeli, Ioannis D. Petsalakis, Mire Zloh "β-Nitroso-o-Quinone Methides: Potent Intermediates in Organic Chemistry and Biology. The impact of the NO group on their Structure and Reactivity Profile. A Theoretical Insight", Structural Chemistry 25,1711 \(2014\)](#)
- [140. I.D.Petsalakis, G.Theodorakopoulos and J.Whitten , "Electronic structure and spectra of \(Cu₂O\) n–H₂O complexes ", Phys. Chem. Chem. Phys., 17,428,\(2015\)](#)
- [141. Demeter Tzeli, Petros G Tsoungas, Ioannis D Petsalakis, Paweł, Kozieliwicz, Mire Zloh, "Intramolecular Cyclization of β-Nitroso-o-Quinone Methides. A Theoretical Endoscopy of a Potentially Useful Innate "Reclusive" Reaction." Tetrahedron, 71, 356, \(2015\)](#)

- [142. Ioannis D. Petsalakis, Giannoula Theodorakopoulos, Omri Buchman, Roi Baer, "Applicability of Mulliken's formula for photoinduced and intramolecular charge-transfer energies", Chem. Phys. Let. 625, 98-103, \(2015\)](#)
- [143. Demeter Tzeli, Ioannis D. Petsalakis, Giannoula Theodorakopoulos, Julius Rebek, Jr, "Reversible encapsulation in a covalent capsule" Chem. Phys. Let. 633, 99-104, \(2015\)](#)
- [144. Demeter Tzeli, Ioannis D. Petsalakis, Giannoula Theodorakopoulos, Julius Rebek, Jr, "Encapsulation of monomers, homodimers and heterodimers of amides and carboxylic acids in three non-covalent assemblies" Struct. Chem. 26,1585-1601, \(2015\)](#)
- [145. A. Stergiou, H. B. Gobeze, I. D. Petsalakis, S. Zhao, H. Shinohara, F. D'Souza and N. Tagmatarchis "Oligothiophene/graphene supramolecular ensembles managing light induced processes: preparation, characterization, and femtosecond transient absorption studies leading to charge-separation", Nanoscale 7,15840-15851, \(2015\)](#)
- [146. Gavette Jesse, Petsalakis Ioannis, Theodorakopoulos Giannoula, Zhang Kang-D, Rebek, Julius, "The Effects of Hexafluoroisopropanol on Guest binding by Water-Soluble Capsules and Cavitand hosts" Chem. Communication, 51 17604-17606, \(2015\)](#)
- [147. Ioannis S.K. Kerkines, Nektarios N. Lathiotakis, Giannoula Theodorakopoulos, Ioannis D. Petsalakis, "Tailoring the spacer type and length in push-pull chromophores. Insights from a systematic theoretical study" Chem. Phys. Let. 653,178-183, \(2016\)](#)
- [148. Demeter Tzeli, Ioannis D. Petsalakis and Giannoula Theodorakopoulos, 'Molecular logic gates based on benzo-18-crown-6 ether of styrylquinoline: a theoretical study' PCCP 18, 32132-32145, \(2016\)](#)
- [149. Nektarios N. Lathiotakis, Giannoula Theodorakopoulos and I. D. Petsalakis 'Electron transfer through organic molecular wires: A theoretical study' Chem.Phys.Let.,667, 45-50, \(2017\)](#)
- [150. Demeter Tzeli, Petros G. Tsoungas, Ioannis D. Petsalakis, a Paweł Kozieliwicz 'Intramolecular Single H bonding vs Bifurcation in Tuning the Conformation of 2,2'-Dihydroxybenzophenone and its Derivatives. A DFT Insight.', Structural Chemistry \(on line 2016\)](#)
- [151. Kumaresh Ghosh, Debojyoti Tarafdar, I.D.Petsalakis and G.Theodorakopoulos, 'Pyridinium urea coupled polyether receptor for selective sensing of Lysine and cell imaging', Eur. J. Org. Chem. 2017, 355-362, \(2017\)](#)
- [152. Luis Martín-Gomis, Nikos. Karousis, Fernando Fernández-Lázaro, Ioannis D. Petsalakis, Kei Ohkubo, Shunichi Fukuzumi, Nikos Tagmatarchis and Ángela Sastre-Santos, "Exfoliation and supramolecular functionalization of graphene with an electron donor perylenediimide derivative", \(2017\)](#)