

Papers in Refereed Journals

2012

1. "Molecular orbital assistance in the design of intramolecular and photoinduced electron transfer systems",
I.D.Petsalakis and G.Theodorakopoulos
Chem. Phys.Lett., 525,105-109 (2012)
[DOI:10.1016/j.cplett.2012.01.002](https://doi.org/10.1016/j.cplett.2012.01.002)
2. "Plasmon-induced enhancement of nonlinear optical rectification in organic materials",
I.Thanopoulos, E. Paspalakis, and V. Yannopoulos,
Phys. Rev. B 85, 035111 (2012)
[DOI: 10.1103/PhysRevB.85.035111](https://doi.org/10.1103/PhysRevB.85.035111)
3. "Theoretical Elucidation of a Classic Reaction: Protonation of the Quadruple Bond of the Octachlorodimolybdate(II,II) [Mo(2)Cl(8)](4-) Anion",
E. D. Simandiras, M. Tsakiroglou, N. Psaroudakis, D. G. Liakos, K. Mertis,
Inorg. Chem. 51, 258 (2012).
[DOI: 10.1021/ic2016325](https://doi.org/10.1021/ic2016325)
4. "Conformations and fluorescence of encapsulated stilbene"
D.Tzeli, G. Theodorakopoulos, I. D. Petsalakis, Dariush Ajami and Julius Rebek, Jr
J. Amer. Chem. Soc., in press
[DOI: 10.1021/ja211164b](https://doi.org/10.1021/ja211164b)
5. "Theoretical study of free and encapsulated carboxylic acid and amide dimers"
D.Tzeli, G. Theodorakopoulos, I. D. Petsalakis, Dariush Ajami and Julius Rebek, Jr
Int. J. Quant. Chem. (in press)
[DOI: 10.1002/qua.24062](https://doi.org/10.1002/qua.24062)
6. "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)
[DOI: 10.1103/PhysRevA.85.032504](https://doi.org/10.1103/PhysRevA.85.032504)
7. "Correlation measures as benchmarks in Reduced Density Matrix Functional Theory",
N. N. Lathiotakis,
Int. J. Quant. Chem. (in press)
[DOI: 10.1002/qua.24069](https://doi.org/10.1002/qua.24069)

2011

1. "Excited state intramolecular proton transfer in hydroxy oxime-based chemical sensors"
I. S. K. Kerkines, I. D. Petsalakis, G. Theodorakopoulos and J. Rebek, Jr,
J. Phys. Chem. A. 115, 834 (2011)
[DOI.org/10.1021/jp1088433](https://doi.org/10.1021/jp1088433)
2. "Theoretical investigation of the complexation of crown ethers and crown ethers of fulleropyrrolidine with $(\text{CH}_3)_x \text{NH}^{4-x}$, $x = 0 - 4$ "
D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos,
Phys.Chem.Chem.Phys. 13, 954 (2011)
[DOI: 10.1039/c0cp00180e](https://doi.org/10.1039/c0cp00180e)
3. "Theoretical study on the electronic structure and the absorption spectra of complexes of C_{60} and C_{59}N with π -extended derivatives of tetrathiafulvalene"
I. D. Petsalakis, D. Tzeli, Ioannis S. K. Kerkines and G. Theodorakopoulos ,
Comp. and Theor. Chem. 965, 168 (2011)
[DOI:10.1016/j.comptc.2011.01.041](https://doi.org/10.1016/j.comptc.2011.01.041)
4. "Photoinduced charge transfer in heterofullerene-donor hybrids: A theoretical study "
I. Thanopoulos, I. D. Petsalakis, and Giannoula Theodorakopoulos,
Chem.Phys.Let. 506, 248 (2011)
[DOI:10.1016/j.cplett.2011.03.028](https://doi.org/10.1016/j.cplett.2011.03.028)
5. "Theoretical calculations on the potential energy curves of electronic states of CF Rydberg states of CF above the lowest ionization limit"
I. D. Petsalakis and G. Theodorakopoulos
Chem. Phys.Lett. 508, 17 (2011)
[DOI:10.1016/j.cplett.2011.04.014](https://doi.org/10.1016/j.cplett.2011.04.014)
6. "Electronic structure and absorption spectra of supramolecular complexes of a fullerene crown ether with a π -extended TTF derivative"
D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos
Phys. Chem. Chem. Phys. 13, 11965 (2011)
[DOI: 10.1039/c0cp02665d](https://doi.org/10.1039/c0cp02665d)
7. "Experimental and theoretical anion binding studies on coumarin linked thiourea and urea molecules "
K. Ghosh, S. Adhikari, R. Fröhlich, I. D. Petsalakis, G. Theodorakopoulos
J. Mol. Structure 1004, 193 (2011)
[DOI:10.1016/j.molstruc.2011.08.004](https://doi.org/10.1016/j.molstruc.2011.08.004)
8. "Fluorescence properties of organic dyes: Quantum chemical studies on the green/blue neutral and protonated DMA-DPH emitters in polymer matrices"
I.S. K. Kerkines, I. D. Petsalakis, G. Theodorakopoulos and P.Argitis
Phys. Chem. Chem. Phys. 13, 21273, (2011)

[DOI: 10.1039/c1cp22499a](https://doi.org/10.1039/c1cp22499a)

9. "Computational insight into the electronic structure and absorption spectra of Lithium complexes of N-confused porphyrin"
D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos,
J. Phys. Chem A 115, 11749 (2011)
[DOI:10.1021/jp204298q](https://doi.org/10.1021/jp204298q)
10. "Theoretical study of hydrogen bonding in homodimers and heterodimers of amide, boronic acid and carboxylic acid, free and in encapsulation complexes"
D.Tzeli, G. Theodorakopoulos, I. D. Petsalakis, Dariush Ajami and Julius Rebek, Jr
J. Amer. Chem.Soc., 133, 16977 (2011)
[DOI:10.1021/ja206555d](https://doi.org/10.1021/ja206555d)
11. "Li atoms attached to helium nanodroplets"
A. Hernando, R. Mayol, M. Pi, M. Barranco, I. S. K. Kerkines, and A. Mavridis,
Int. J. Quantum Chem., 111, 400 (2011)
[DOI:10.1002/qua.22636](https://doi.org/10.1002/qua.22636)
12. "Enhancement of ultraviolet photo-induced energy transfer near plasmonic nanostructures"
I. Thanopoulos, E. Paspalakis, and V. Yannopapas,
J. Phys. Chem. C 115, 4370-4374 (2011)
[DOI: 10.1021/jp106564c](https://doi.org/10.1021/jp106564c)
13. "Outer-valence Green's function method using natural orbitals for ultrafast electron dynamics",
I.Thanopoulos,
Comp. Theor. Chem. 970, 42 (2011)
[DOI: 10.1016/j.comptc.2011.05.0241](https://doi.org/10.1016/j.comptc.2011.05.0241)
14. "Fractional spin in reduced density-matrix functional theory",
N. Helbig, G. Theodorakopoulos, and N. N. Lathiotakis,
J. Chem. Phys. 135, 054109 (2011)
[DOI: 10.1063/1.3615955](https://doi.org/10.1063/1.3615955)

2010

1. "Coherent oscillatory femtosecond dynamics in multichannel photodynamics of NO₂ studied by spatially masked electron imaging",
D. Irimia, I. D. Petsalakis, G. Theodorakopoulos, and M. H. M. Janssen,
J. Phys. Chem. A 114, 3157 (2010).
[DOI: 10.1021/jp909031p](https://doi.org/10.1021/jp909031p)
2. "*trans*-pyridyl and naphthyridyl cinnamides as alternatives for urea in complexation of carboxylic acid and formation of water-templated assemblies in the solid state",

- K. Ghosh, T. Sen, R. Froehlich, I. D. Petsalakis, and G. Theodorakopoulos,
J. Phys. Chem. B **114**, 321 (2010).
[DOI: 10.1021/jp907521j](https://doi.org/10.1021/jp907521j)
3. “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 and 4-(dicyanomethylene)-2-methyl-6-p-(dimethyl-amino) styryl-4H-pyran, by DFT and TDDFT calculations”,
I. D. Petsalakis, D. G. Georgiadou, M. Vasilopoulou, G. Pistolis, D. Dimotikali, P. Argitis, and G. Theodorakopoulos,
J. Phys. Chem. A **114**, 5580 (2010).
[DOI: 10.1021/jp100338d](https://doi.org/10.1021/jp100338d)
 4. “Size consistency of explicit functionals of the natural orbitals in reduced density matrix functional theory”,
N. N. Lathiotakis, N. I. Gidopoulos, and N. Helbig,
J. Chem. Phys. **132**, 084105 (2010).
[DOI: 10.1063/1.3324699](https://doi.org/10.1063/1.3324699)
 5. “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,
Zeit. Phys. Chem. **224**, 467 (2010).
[DOI: 10.1524/zpch.2010.6118](https://doi.org/10.1524/zpch.2010.6118)
 6. “Coherence effects in laser-induced continuum structure”,
I. Thanopoulos and M. Shapiro,
Adv. Quan. Chem. **60**, 105 (2010).
[DOI: 10.1016/S0065-3276\(10\)60003-2](https://doi.org/10.1016/S0065-3276(10)60003-2)
 7. “Intermolecular energy transfer dynamics 24-mode pyrazine by partitioning technique: A time-dependent approach”,
I. Thanopoulos, P. Brumer, and M. Shapiro,
J. Chem. Phys. **133**, 154111 (2010).
[DOI: 10.1063/1.3495953](https://doi.org/10.1063/1.3495953)
 8. “Accurate ab initio calculations of the ground states of FeC, FeC⁺, and FeC⁻”,
D. Tzeli and A. Mavridis,
J. Chem. Phys. **132**, 194312 (2010).
[DOI: 10.1063/1.3429612](https://doi.org/10.1063/1.3429612)
 9. “Mind the basis set superposition error”,
D. Tzeli and A. A. Tsekouras,
Chem. Phys. Lett. **496**, 42 (2010).
[DOI: 10.1016/j.cplett.2010.07.053](https://doi.org/10.1016/j.cplett.2010.07.053)
 10. “Experimental and theoretical study of the reaction of POCl₃⁻ with O₂”,
I. S. K. Kerkines, K. Morokuma, N. Iordanova, and A. A. Viggiano,
J. Chem. Phys. **132**, 044309 (2010).

[DOI: 10.1063/1.3299276](https://doi.org/10.1063/1.3299276)

2009

11. “Discontinuity of the chemical potential in reduced-density-matrix-functional theory for open-shell systems”,
N. Helbig, N. N. Lathiotakis, E. K. U. Gross,
Phys. Rev. A 79, 022504 (2009).
[DOI: 10.1103/PhysRevA.79.022504](https://doi.org/10.1103/PhysRevA.79.022504)
12. “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, and E. K. U. Gross,
J. Chem. Phys, 130, 064109 (2009).
[DOI: 10.1063/1.3073053](https://doi.org/10.1063/1.3073053)
13. “Density-Matrix-Power Functional: Performance for finite systems”,
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 (2009).
[DOI: 10.1103/PhysRevA.79.040501](https://doi.org/10.1103/PhysRevA.79.040501)
14. “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).
[DOI: 10.1039/b902278c](https://doi.org/10.1039/b902278c)
15. “Optical Control of Molecular Switches”,
I. Thanopoulos, P. Kral, M. Shapiro, and E. Paspalakis,
J. Mod. Opt. 56, 686 (2009).
[DOI:10.1080/09500340802326815](https://doi.org/10.1080/09500340802326815)
16. “Preface: Special Issue on Quantum Control of Matter and Light”,
E. Paspalakis and I. Thanopoulos,
J. Mod. Opt. 56 , 685 (2009).
[DOI: 10.1080/09500340802547501](https://doi.org/10.1080/09500340802547501)
17. “Theoretical study of adsorption of group IIIA nitrides on Si(111)”,
D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos,
J. Phys. Chem. C 113, 5563 (2009).
[DOI: 10.1021/jp810838s](https://doi.org/10.1021/jp810838s)
18. “Electron inelastic mean free paths in biological matter based on dielectric theory and local-field corrections”,
D. Emfietzoglou , I. Kyriakou, I. Abril, R. Garcia-Molina, I.D. Petsalakis, H. Nikjoo, A. Pathak,
Nucl. Instr. and Meth. B 267, 45 (2009).
[DOI: 10.1016/j.nimb.2008.11.008](https://doi.org/10.1016/j.nimb.2008.11.008)

19. "Triphenylamine-based receptors in selective recognition of dicarboxylic acids",
K. Ghosh, G. Masanta, R. Fröhlich, I. D. Petsalakis and G. Theodorakopoulos,
J. Phys. Chem. B 113, 7800 (2009).
[DOI: 10.1021/jp901151w](https://doi.org/10.1021/jp901151w)
20. "Emitting and electron-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).
[DOI: 10.1016/j.cplett.2009.04.080](https://doi.org/10.1016/j.cplett.2009.04.080)
21. "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. Nanotechnol. 6, 164 (2009).
[DOI: 10.1504/IJNT.2009.021714](https://doi.org/10.1504/IJNT.2009.021714)
22. "Theoretical Study of Adsorption and Diffusion of Group IIIA Metals on Si(111)",
D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos,
J. Phys. Chem. C, in press (2009).
[DOI: 10.1021/jp903389r](https://doi.org/10.1021/jp903389r)

2008

13. "Semi-empirical dielectric descriptions of the Bethe surface of the valence bands of condensed water",
D. Emfietzoglou, I. Abril, R. Garcia-Molina, I.D. Petsalakis, H. Nikjoo and A. Pathak,
Nucl. Instr. and Meth. B 266, 1154 (2008).
[DOI: 10.1016/j.nimb.2007.11.057](https://doi.org/10.1016/j.nimb.2007.11.057)
14. "Structure and energetics of InN and GaN dimers",
L. Šimová, D. Tzeli, M. Urban, I. Černušák, G. Theodorakopoulos and I.D. Petsalakis,
Chem. Phys. 349, 98 (2008).
[DOI: 10.1016/j.chemphys.2008.02.051](https://doi.org/10.1016/j.chemphys.2008.02.051)
15. "Theoretical study on the electronic states of NaLi",
I.D. Petsalakis, D. Tzeli and G. Theodorakopoulos,
J. Chem. Phys. 129, 054306 (2008).
[DOI: 10.1063/1.2956510](https://doi.org/10.1063/1.2956510)
16. "Theoretical study of gallium nitride molecules GaN₂ and GaN₄",
D. Tzeli, G. Theodorakopoulos and I.D. Petsalakis,
J. Phys. Chem. A 112, 8858 (2008).
[DOI: 10.1021/jp8019396](https://doi.org/10.1021/jp8019396)

17. "First principles study of the electronic structure and bonding of Mn_2 ",
D. Tzeli, U. Miranda, I.G. Kaplan and A. Mavridis,
J. Chem. Phys. 129, 154310 (2008).
[DOI:10.1063/1.2993750](https://doi.org/10.1063/1.2993750)
18. "Theoretical study on tertiary amine-fluorophore photoinduced transfer (PET) systems",
I.D. Petsalakis, N.N. Lathiotakis and G. Theodorakopoulos,
J.Mol. Struct. (Theochem.) 867, 64 (2008).
[DOI: 10.1016/j.theochem.2008.07.025](https://doi.org/10.1016/j.theochem.2008.07.025)
19. "Photoinduced charge transfer in fullerene-donor dyads: A theoretical study",
I.D. Petsalakis and G. Theodorakopoulos,
Chem. Phys. Let. 466, 189 (2008).
[DOI: 10.1016/j.cplett.2008.10.058](https://doi.org/10.1016/j.cplett.2008.10.058)
20. "Empirical functionals in reduced-density-matrix-functional theory",
M.A.L. Marques and N.N. Lathiotakis,
Phys. Rev. A 77, 032509 (2008).
[DOI: 10.1103/PhysRevA.77.032509](https://doi.org/10.1103/PhysRevA.77.032509)
21. "Benchmark calculations for reduced density matrix functionals",
N.N. Lathiotakis and M.A.L. Marques,
J. Chem. Phys. 128, 184103 (2008).
[DOI: 10.1063/1.2899328](https://doi.org/10.1063/1.2899328)
22. "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).
[DOI: 10.1103/PhysRevB.78.201103](https://doi.org/10.1103/PhysRevB.78.201103)
23. "Codoping: A possible pathway for inducing ferromagnetism in ZnO",
N.N. Lathiotakis, A.N. Andriotis and M. Menon,
Phys. Rev. B 78, 193311 (2008).
[DOI: 10.1103/PhysRevB.78.193311](https://doi.org/10.1103/PhysRevB.78.193311)
24. "Electronic structure and bonding of the 3d-transition metal borides, MB, M = Sc, Ti, V, Cr, Mn, Fe, Co, Ni, and Cu through all electron *ab initio* calculations", D. Tzeli and A. Mavridis,
J. Chem. Phys. 128, 034309 (2008).
[DOI: 10.1063/1.2821104](https://doi.org/10.1063/1.2821104)
25. "The electron affinity of the gallium nitride GaN and digallium nitride, GaNGa. The importance of the basis set superposition error in strongly bound systems",
D. Tzeli and A.A. Tsekouras,
J. Chem. Phys. 128, 144103 (2008).
[DOI: 10.1063/1.2883997](https://doi.org/10.1063/1.2883997)

26. "Structural properties of lithium metaphosphate glasses by ab initio molecular electronic structure calculations",
D.G. Liakos and E.D. Simandiras,
J. Non-Cryst. Solids **354**, 1569 (2008).
[DOI: 10.1016/j.jnoncrysol.2007.08.077](https://doi.org/10.1016/j.jnoncrysol.2007.08.077)
27. "Theoretical study of glass systems using molecular electronic structure theory. 2. Structure and spectroscopy of the B₂O₃ glass",
D.G. Liakos and E.D. Simandiras,
J. Phys. Chem. A, **112**, 7881 (2008).
[DOI: 10.1021/jp711332k](https://doi.org/10.1021/jp711332k)
28. "Optical switching of electric charge transfer pathways in porphyrin: A light-controlled nanoscale current router",
I. Thanopoulos, E. Paspalakis and V. Yannopoulos,
Nanotechnology **19**, 445202 (2008).
[DOI: 10.1088/0957-4484/19/44/445202](https://doi.org/10.1088/0957-4484/19/44/445202)
29. "Coarse grained open system quantum dynamics",
I. Thanopoulos, P. Brumer and M. Shapiro,
J. Chem. Phys. **129**, 194104 (2008).
[DOI: 10.1063/1.3010370](https://doi.org/10.1063/1.3010370)

2007

30. "Theoretical study of nonadiabatic interactions, radiative lifetimes and predissociation lifetimes of excited states of BH",
I.D. Petsalakis and G. Theodorakopoulos,
Molecular Physics **105**, 333 (2007).
[DOI: 10.1080/00268970601110308](https://doi.org/10.1080/00268970601110308)
31. "Theoretical study on triphenylamine-based sensors of dicarboxylic acids",
I.D. Petsalakis, N. Tagmatarchis, G. Rotas and G. Theodorakopoulos,
J. Molecular Structure: THEOCHEM **807**, 11 (2007).
[DOI: 10.1016/j.theochem.2006.12.008](https://doi.org/10.1016/j.theochem.2006.12.008)
32. "A consistent dielectric response model for water ice over the whole energy-momentum plane",
D. Emfietzoglou, H. Nikjoo, I.D. Petsalakis and A. Pathak,
Nuclear Instruments and Methods in Physics Research B **256**, 141 (2007).
[DOI: 10.1016/j.nimb.2006.11.105](https://doi.org/10.1016/j.nimb.2006.11.105)
33. "Theoretical study of fulleropyrrolidines by density functional and time-dependent density functional theory",
I.D. Petsalakis, N. Tagmatarchis and G. Theodorakopoulos,
J. Phys. Chem. C **111**, 14139 (2007).
[DOI: 10.1021/jp0743774](https://doi.org/10.1021/jp0743774)

34. "Theoretical investigation on the electronic and geometric structure of GaN_2^+ and GaN_4^+ ",
D. Tzeli, I.D. Petsalakis and G. Theodorakopoulos,
J. Phys. Chem. A **111**, 8892 (2007).
[DOI: 10.1021/jp074313t](https://doi.org/10.1021/jp074313t)
35. "Theoretical study of adsorption of gallium and gallium nitrides on Si(111)",
D. Tzeli, I.D. Petsalakis and G. Theodorakopoulos,
Chem. Phys. Lett. **448**, 88 (2007).
[DOI: 10.1016/j.cplett.2007.09.060](https://doi.org/10.1016/j.cplett.2007.09.060)
36. "Theoretical study in donor-acceptor carbon nanohorn-based hybrids",
I.D. Petsalakis, G. Pagona, N. Tagmatarchis and G. Theodorakopoulos,
Chem. Phys. Lett. **448**, 115 (2007).
[DOI: 10.1016/j.cplett.2007.09.067](https://doi.org/10.1016/j.cplett.2007.09.067)
37. "Improved theoretical calculations of InN in its $X^3\Sigma^-$ ground state and in the first $^3\Pi$ excited state",
L. Demovič, I. Černušák, G. Theodorakopoulos, I.D. Petsalakis and M. Urban,
Chem. Phys. Lett. **447**, 215 (2007).
[DOI: 10.1016/j.cplett.2007.09.035](https://doi.org/10.1016/j.cplett.2007.09.035)
38. "Theoretical investigation of the stepwise hydrolysis of the $[\text{Re}_3(-\text{Cl})_3\text{Cl}_9]^{3-}$ Anion",
D.G. Liakos, E.D. Simandiras, N. Psaroudakis and K. Mertis,
Inorg. Chem., **46**, 2167 (2007).
[DOI: 10.1021/ic061862p](https://doi.org/10.1021/ic061862p)
39. "Electron-transfer on aqueous photoactive carbon nanohorn-pyrene-tetrathiafulvalene hybrids",
G. Pagona, A.S.D. Sandanayaka, A. Maigné, J. Fan, G.C. Papavassiliou, I.D. Petsalakis, B.R. Steele, N. Tagmatarchis, M. Yudasaka, S. Iijima and O. Ito,
Chem. Eur. J. **13**, 7600 (2007).
[DOI: 10.1002/chem.200700639](https://doi.org/10.1002/chem.200700639)
40. "Soluble functionalized carbon nanohorns",
G. Pagona, G. Rotas, I.D. Petsalakis, G. Theodorakopoulos, A. Maigné, J. Fan, M. Yudasaka, S. Iijima and N. Tagmatarchis,
J. Nanosci. Nanotechnol. **7**, 3468 (2007).
[DOI: 10.1166/jnn.2007.821](https://doi.org/10.1166/jnn.2007.821)

2006

41. "Multireference configuration interaction and quantum defect calculations on the Rydberg states of the BH molecule",
I.D. Petsalakis and G. Theodorakopoulos,
Mol. Phys. **104**, 103 (2006).

42. "Quasi-molecular radiative transitions produced by thermal and low-temperature collisions: $\text{Ar}(3p^6\ ^1S_0 - 3p^54s\ ^3P_2) - \text{He}$ ",
A. Devdariani, E. Chesnokov, A. Zagrebin, M.G. Lednev, I.D. Petsalakis, G. Theodorakopoulos, H.P. Liebermann and R.J. Buenker,
Chem. Phys. 330, 101 (2006).
43. "Unbalanced strain-directed functionalization of carbon nanohorns: A theoretical investigation based on complementary methods",
I.D. Petsalakis, G. Pagona, G. Theodorakopoulos, N. Tagmatarchis, M. Yudasaka, and S. Iijima,
Chem. Phys. Lett. 429, 194 (2006).
44. "Theoretical study on the low-lying electronic states of InN ",
G. Theodorakopoulos and I. D. Petsalakis,
Chem. Phys. Lett. 423, 445 (2006).

2005

45. "Theoretical study of benzene, toluene and dibromobenzene at a $\text{Si}(111)\ 7\times 7$ surface",
I.D. Petsalakis, J.C. Polanyi and G. Theodorakopoulos,
Israel J. Chemistry 45, 111 (2005).
46. "Theoretical study of halogen-substituted benzene on a $\text{Si}(111)\ 7\times 7$ surface",
I.D. Petsalakis and G. Theodorakopoulos,
Israel J. Chemistry 45, 127 (2005).
47. "Generation of the $\text{C}_2\text{H}_3\text{O}^+$ ion in reactions of $\text{O}(\text{P}_3)$ with 2-butyne",
A. Metropoulos,
Int. J. Quantum Chem. 104, 482 (2005).
48. "Description of the lowest-energy surfaces of the $\text{CH}+\text{O}$ 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 (2005).

2004

49. "Theoretical ab initio study on the electronic states of GaO and Ga_2O ",
I. D. Petsalakis, G. Theodorakopoulos, R.W. Gora and S. Roszak,
J. Mol. Struct. (Theochem.) 672, 105 (2004).
50. "Parent- and daughter-mediated halogenation reactions modeled for 1,2- and 1,4-dibromobenzene $\text{Si}(111)\text{-}7\times 7$ ",

R. K. Harikumar, I. D. Petsalakis, J. C. Polanyi, and G. Theodorakopoulos, *Surface Science* 572, 162 (2004).

51. "An ab initio study of the ground states of the vinoxy radical and of its ion",
A. Metropoulos,
J. Mol. Struct. (Theochem) 674, 19 (2004).
52. "Theoretical study of glass systems using ab initio molecular electronic structure theory. 1. Lithium metaphosphate glass",
E. D. Simandiras and D. G. Liakos,
J. Phys. Chem. A 108, 3854 (2004).

53.

2003

53. "Broadband absorption and ab initio results on the $CF\ C^2\Sigma^+ - X^2\Pi$ system",
J. Luque, E.A. Hudson, J.P. Booth and I.D. Petsalakis,
J. Chem. Phys. 118, 1206 (2003).
54. "Theoretical ab initio study of the electronic states of KrH and KrH^+ . Quantum defect and complex coordinate calculations on the Rydberg states of KrH ",
I.D. Petsalakis, G. Theodorakopoulos and R.J. Buenker,
J. Chem. Phys. 119, 2004 (2003).
55. "Theoretical study of the induced attachment of benzene to $Si(111) 7\times 7$ ",
I.D. Petsalakis, J.C. Polanyi and G. Theodorakopoulos,
Surface Science 544, 162 (2003).
56. "States of the CH_3C radical conducive to the formation of the $C_2H_3O^+$ ion",
A. Metropoulos,
Chem. Phys. Lett. 368, 701 (2003).
57. "A possible pathway for the formation of the $C_2H_3O^+$ chemi-ion",
A. Metropoulos,
Chem Phys. Lett. 375, 26 (2003).
58. "Ab initio investigation of the ground state properties of PO , PO^+ , and PO^- ",
A. Metropoulos, A. Papakondylis and A. Mavridis,
J. Chem. Phys. 119, 5981 (2003).
59. "On the feasibility of chemi-ion formation in the system $CH_2CH(\tilde{a}^4A) + O(^3P)$ ",
A. Metropoulos,
J. Chem. Phys. 119, 12029 (2003).
60. "A theoretical study on the solvolytic reactivity of the $[Re_3(\mu-Cl_3)Cl_9]^{n-}$ clusters ($n=3,4$) using ab initio and density functional theory calculations",

N. Psaroudakis, K. Mertis, D. G. Liakos and E. D. Simandiras,
Chem. Phys. Lett. 369, 490 (2003).

2002

61. "Ab initio spin-orbit configuration interaction calculation for potential curves and radiative lifetimes of the low-lying electronic states of Lead monofluoride",
K. Das, I. D. Petsalakis, H. P. Lieberman and R. J. Buenker,
J. Chem. Phys. 116, 608 (2002).
62. "On the construction and use of ab initio quantum defect functions for the Rydberg spectra of molecules",
G. Theodorakopoulos, I. D. Petsalakis and M. S. Child,
Rus. J. Phys. Chem. 76, S95 (2002).
63. "Complex coordinate calculations on predissociating states of diatomic molecules",
I. D. Petsalakis, G. Theodorakopoulos and R. J. Buenker,
Rus. J. Phys. Chem. 76, S1 (2002).
64. "Potential energy curves and dipole transition moments for excited electronic states of XeKr and ArNe",
I. D. Petsalakis, G. Theodorakopoulos, H. P. Lieberman and R. J. Buenker,
J. Chem. Phys. 117, 3639 (2002).
65. "The ab initio potential energy surface and vibration-rotation energy levels of $X^2\Sigma^+ MgOH$ ",
J. Koput, S. Carter, K. A. Peterson and G. Theodorakopoulos,
J. Chem. Phys. 117 1529 (2002).
66. "Ab initio calculations on electronic states of CaOH",
G. Theodorakopoulos, I. D. Petsalakis, H. P. Lieberman, R. J. Buenker and J. Koput,
J. Chem. Phys. 117, 4810 (2002).
67. "The importance of the diabatic channels to the chemi-ionization reaction $O(^3P) + CH(a^4\Sigma^-) \rightarrow HCO^+(X^1\Sigma^+) + e^-$ ",
A. Metropoulos,
J. Chem. Phys. 116, 6376 (2002).
68. "An accurate description of the ground and excited states of SiH",
A. Kalemou, A. Mavridis and A. Metropoulos,
J. Chem. Phys. 116, 6529 (2002).

2001

69. "Potential energy curves and dipole transition moments for electronic states of ArHe and HeNe",
I. D. Petsalakis, H. P. Lieberman, R. J. Buenker and G. Theodorakopoulos,
J. Chem. Phys. 115, 6365 (2001).

70. "The Rydberg states of NO₂. Vibrational autoionization of the ndσ states",
I. D. Petsalakis, G. Theodorakopoulos and M. S. Child,
J. Chem. Phys. 115, 10394 (2001).
71. "Conditions conducive to the chemi-ionization reaction O(³P)+CH(X²Π,
a⁴Σ⁻) → HCO⁺(X¹Σ⁺) + e⁻",
A. Metropoulos and A. Mavridis,
J. Chem. Phys. 115, 6946 (2001).

2000

72. "Electronic states of CF⁺",
I. D. Petsalakis, G. Theodorakopoulos,
Chem. Phys. 254, 181 (2000).
73. "Potential energy curves and dipole transition moments to the ground state
of the system Ar^{*}(3p⁵4s, ³P, ¹P) + Ne",
I. D. Petsalakis, R. J. Buenker, H. P. Lieberman, A. B. Alekseyev, A. Z.
Devdariani and G. Theodorakopoulos,
J. Chem. Phys. 113, 5812 (2000).
74. "Predissociation lifetimes of the E ²Π and F ²Π states of CH",
A. Metropoulos and A. Mavridis,
Chem. Phys. Lett. 331, 89 (2000).

1999

75. "An accurate description of the ground and excited states of CH",
A. Kalemou, A. Mavridis and A. Metropoulos,
J. Chem. Phys. 111, 9536 (1999).
76. "Complex coordinate calculations on autoionizing states of HeH and H₂",
M. Honigmann, G. Hirsch, R. J. Buenker, I. D. Petsalakis and G.
Theodorakopoulos,
Chem. Phys. Lett. 305, 465 (1999).
77. "Ab initio calculations on the ground and excited states of BeOH and
MgOH",
G. Theodorakopoulos, I. D. Petsalakis and I. P. Hamilton,
J. Chem. Phys. 111, 10484 (1999).
78. "Theoretical study on electronic states of carbon monofluoride and on the
predissociation of the lower lying state",
I. D. Petsalakis,
J. Chem. Phys. 110, 10730 (1999).
79. "Theoretical calculations on the linewidths of rovibrational levels of the 3d
Rydberg states of BeH and BeD",
I. D. Petsalakis, D. Papadopoulos, G. Theodorakopoulos and R. J. Buenker,
J. Phys. B 32, 3225 (1999).

1998

80. "Dynamics of on the ground-state potential surfaces of H₃ and its isotopomeres from their uv spectra",
D. Azinovic, R. Bruckmeier, Ch. Wunderlich, H. Figger, G. Theodorakopoulos and I. D. Petsalakis,
Phys. Rev. A 58, 1115 (1998).
81. "Theoretical study on the Rydberg states of NeH: Ab initio quantum defect and complex coordinate calculation",
I. D. Petsalakis, G. Theodorakopoulos, Y. Li, G. Hirsch, R.J. Buenker and M.S. Child,
J. Chem. Phys. 108, 7607 (1998).
82. "An ab initio potential energy surface and spectroscopic constants for the X¹Σ_g⁺ state of NO₂⁺",
G. Theodorakopoulos, I. D. Petsalakis and M. S. Child,
J. Molecular Structure (Theochem) 434, 177 (1998).

1997

83. "Ab initio configuration interaction calculations of the predissociation of rovibrational levels of the C ³Π_g and the d ¹Π_g 3σ Rydberg states of the oxygen molecule",
Y. Li, I. D. Petsalakis, H. P. Liebermann, G. Hirsch and R. J. Buenker,
J. Chem. Phys. 106, 1123 (1997).
84. "The effect of correlation on the Jahn -Teller instability of cyclobutadiene",
A. Metropoulos and Y. N. Chiu,
J. Mol. Struct. (Theochem) 417, 95 (1997).
85. "Complex L² calculation of HOCO resonances",
J. Bowman and A. Metropoulos,
J. Chem. Soc. Faraday Trans. 93, 815 (1997).
86. "Predissociation widths and lifetimes of the n=3 ²Σ⁺ states of BeH",
I. D. Petsalakis, R. J. Buenker, G. Hirsch and G. Theodorakopoulos,
J. Phys. B 30, 4935 (1997).

1996

87. "On the construction and use of ab initio quantum defect functions for H₂O",
G. Theodorakopoulos, I. D. Petsalakis and M. S. Child,
J. Phys. B At. Mol. Opt. Phys. 29 , 4543 (1996).
88. "Further Exploration of C₄H₄",
A. Metropoulos and Y. N. Chiu,
J. Mol. Struct. (Theochem) 365, 119 (1996).

89. "Prediction of nonclassical hydrogen complexes of nontransition metals",
C. A. Nicolaides and E. D. Simandiras,
Comments Inorg. Chem. 18, 65 (1996).

Papers in Conference Proceedings

90. "A DFT study of adsorption of gallium and gallium nitrides on Si(111)",
D. Tzeli, G. Theodorakopoulos and I.D. Petsalakis,
Frontiers in Quantum Systems in Chemistry and Physics – PTCP 18, 341
(2008), Proceedings of the QCSP-XII, Ed. S. Wilson et al. Springer Science.
91. "Lowest energy path of oxygen near CH: A combined configuration
interaction and Tight-Binding approach",
N. C. Bacalis, A. Metropoulos, D. A. Papaconstantopoulos,
Int. Conf. Computational Meth. Sci. and Eng., Athens (2004), Lecture Series
on Computer and Computational Sciences, Vol 1, pp 1015-1021 (2004).
92. "Theoretical ab initio study of radiative transitions of Xe*-Kr",
I. D. Petsalakis, G. Theodorakopoulos and R. J. Buenker,
in Proceedings of the international seminar on atomic interactions and
differential scattering, St. Andreasberg, Germany, 18-21 March 2002.
<http://www.ampap.uni-hannover.de/is/>
93. "Potential energy surfaces for MOH systems, M=Be,Mg, Ca", G.
Theodorakopoulos, in Proceedings of the international seminar on atomic
interactions and differential scattering, St. Andreasberg, Germany, 18-21
March 2002. <http://www.ampap.uni-hannover.de/is/>

PhD Theses

94. "Theoretical calculations on inorganic materials",
D. Liakos, supervisors E.D. Simandiras and A.T. Tsatsas,
University of Athens, Chemistry Department (2007).