

1. Papers in Refereed Journals

1. "MRD CI calculations on the asymmetric stretch potentials of H₂O in the ground and the first seven singlet excited states ",
G. Theodorakopoulos, I.D. Petsalakis and R.J. Buenker,
Chem. Phys. 96, 217 (1985).
2. "Configuration interaction study of the oscillator strengths for the \tilde{B}^1A_1 -- \tilde{X}^1A_1 and \tilde{D}^1A_1 -- \tilde{X}^1A_1 transitions of the water molecule ",
G. Theodorakopoulos, I.D. Petsalakis, C.A. Nicolaides and R.J. Buenker,
Chem. Phys. 100, 331 (1985).
3. "The $\tilde{X}^1A_1 \rightarrow \tilde{A}^1B_1$ transition moment of H₂O using state-specific configuration-interaction wave functions",
G. Theodorakopoulos, I.D. Petsalakis, C.A. Nicolaides and R.J. Buenker,
J. Chem. Phys. 82, 912 (1985).
4. "The effect of intermolecular interactions on the 2nd hyperpolarizability of the ammonia heptamer",
J. Waite and M.G. Papadopoulos,
Chem. Phys. Lett. 114, 539 (1985).
5. "The effect of intramolecular processes on the polarizabilities and hyperpolarizabilities of some amines",
J. Waite and M.G. Papadopoulos,
J. Chem. Phys. 82, 1427 (1985).
6. "The polarizability and 2nd hyperpolarizability of some azabenzenes",
M.G. Papadopoulos and J. Waite,
J. Chem. Phys. 82, 1435 (1985).
7. "Polarizability and 2nd hyperpolarizability of some molecular cations - the effect of charge variation on these properties",
J. Waite and M.G. Papadopoulos,
J. Phys. Chem. 89, 2291 (1985).
8. "Calculations of induced moments in large molecules - the average polarizability and 2nd hyperpolarizability of some polyacetylenes and a scale of polarization for CH₃, F, H and NH₂ - a comparative study",
J. Waite and M.G. Papadopoulos,
J. Chem. Soc. - Faraday Transactions II 81, 433 (1985).

9. "The effect of structural-changes on the polarizability and 2nd hyperpolarizability in some benzene isomers and their anions",
 J. Waite and M.G. Papadopoulos,
 Z. Naturforsch. A 40, 142 (1985).
10. "A quasiclassical study of collisions of He with HD ($B^1\Sigma_u^+$)",
 S.C. Farantos,
 Mol. Phys. 54, 835 (1985).
11. "Quantum and classical vibrational chaos in floppy molecules",
 S.C. Farantos and J. Tennyson,
 J. Chem. Phys. 82, 800 (1985).
12. "Rovibrational spectrum of the excited potential energy surface of He+H₂ ($B^1\Sigma_u^+$)",
 S.C. Farantos and J. Tennyson,
 J. Chem. Phys. 82, 2163 (1985).
13. "Routes to vibrational chaos in triatomic-molecules",
 J. Tennyson and S.C. Farantos,
 Chem. Phys. 93, 237 (1985).
14. "Multichannel relativistic autoionisation of negative ions: the 1s2s2p³ $^6S_{5/2}^0$ metastable state of Be⁻",
 G. Aspromallis, C.A. Nicolaides and Y. Komninos,
 J. Phys. B 18, L545 (1985).
15. "Partial widths and interchannel coupling in auto-ionizing states in terms of complex eigenvalues and complex coordinates",
 C.A. Nicolaides and T. Mercouris,
 Phys. Rev. A 32, 3247 (1985).
16. "Exchange-energy contribution to the interaction of Helium with a metal-surface",
 A.N. Andriotis,
 Phys. Rev. B 31, 4003 (1985).
17. "Work-function changes due to surface anisotropy and imperfections",
 A.N. Andriotis,
 Phys. Rev. B 32, 5062 (1985).
18. "Preparation and characterization of some new π -Donors - the 3,4,5-Tris(Alkylthio)-1,2-Dithiolium Iodides, Tetrakis(Alkylthio)-1,1',2,2'-Tetrathiafulvalenes, and similar compounds",
 G.C. Papavassiliou,
 Chemica Scripta 25, 167 (1985).
19. "Some new conducting solids",
 G.C. Papavassiliou, E.I. Kamitsos and J.S. Zambounis,

Mol. Cryst. Liq. Cryst. 120, 315 (1985).

20. "Bis (Diazino) tetrathiafulvalenes and similar π -Donors",
G.C. Papavassiliou, S.Y. Yiannopoulos and J.S. Zambounis,
Mol. Cryst. Liq. Cryst. 120, 333 (1985).

21. "Gain measurements at 157 nm in an F_2 pulsed discharge molecular laser",
A.C. Cefalas, C. Skordoulis, M. Kompitsas and C.A. Nicolaides,
Opt. Commun. 55, 423 (1985).

2. Papers in Proceedings of International and National Conferences

1. "Relativistic autoionization in atoms: application to Be^- ",
D.R. Beck and C.A. Nicolaides,
Argonne National Laboratory Report (1985).

2. "Transformation phenomena exhibited by M-TCNQ materials. A resonance Raman study",
E.I. Kamitsos,
Proc. 3rd Greek Conf. on Lasers and Applications, Kolympari, Crete, 1985, pp. 85-87 (in Greek).

3. Dissertations

a. PhD theses

1. "Study of excited states of molecular systems using non-orthonormal electronic configurations",
I.D. Petsalakis, supervisor C.A. Nicolaides, University of Athens (1985).

b. Honors theses

1. "Study of the Kerr effect in crystals",
D. Aggelaki and D. Christopoulos, supervisors A.C. Cefalas and A.A. Serafetinides, National Technical University of Athens (1985).