DEMETER TZELI

PUBLICATIONS –MAY 2009

A. PAPERS IN REFEREED JOURNALS

1. "On the Electronic Structure of the Ground ($X^3\Sigma^-$) and Some Low-Lying States ($A^3\Pi$, $a^1\Delta$, $b^1\Sigma^+$, $B^3\Sigma^-$) of the Isovalent Species P-Li and P-Na", D. Tzeli, A. Papakondylis and A. Mavridis, J. Mol. Struct.(THEOCHEM) **417**, 277 (1997). [DOI: 10.1016/S0166-1280(97)00146-2]

2. "On the Electronic Structure of NLi_2 and PLi_2. Ground and Low-Lying Excited States", D. Tzeli, A. Papakondylis and A. Mavridis, *J. Phys. Chem. A* **102**, 2223 (1998). [DOI: 10.1021/jp972998z]

3. "The electronic structure of $ScAl^+$. Ground and Low-Lying excited states", D. Tzeli and A. Mavridis, *J. Phys. Chem. A*, **104**, 6861 (2000). [DOI: 10.1021/jp000894+]

4. "A first principles study of the acetylene--water interaction", D. Tzeli, A. Mavridis, and S. S. Xantheas, *J. Chem. Phys.* **112**, 6178 (2000). [DOI: 10.1063/1.481268]

5. "First principles investigation of Boron and Aluminum Carbides, BC, AlC and their Anions, BC^- and AlC^-. 1", D. Tzeli and A. Mavridis, *J. Phys. Chem. A*, **105**, 1175, (2001). [DOI: 10.1021/jp003258k]

6. "Accurate Theoretical Study of the Excited States of Boron and Aluminum Carbides, BC, AlC. 2", D. Tzeli and A. Mavridis, *J. Phys. Chem. A*, **105**, 7672 (2001). [DOI: 10.1021/jp010459v]

7. "A molecular level study of the aqueous microsolvation of acetylene", D.Tzeli, A. Mavridis and S. Xantheas, *Chem. Phys. Lett.*, **340**, 538 (2001). [DOI: 10.1016/S0009-2614(01)00444-4]

8. "Theoretical investigation of iron carbide, FeC", D. Tzeli and A. Mavridis, *J. Chem. Phys.* **116**, 4901 (2002). [DOI: 10.1063/1.1450548]

9. "First principles Examination of the Acetylene-Water clusters, HCCH-$(H_2O)_x$, x = 2, 3, and 4", D.Tzeli, A. Mavridis and S. Xantheas, *J. Phys. Chem. A*, **106**, 11327 (2002). [DOI: 10.1021/jp021191q] [Supplorting information]

10. "On the dipole moment of the ground state X $^3\Delta$ of iron carbide, FeC", D. Tzeli and A. Mavridis, *J. Chem. Phys.*, **118**, 4984 (2003). [DOI: 10.1063/1.1545680]

11. "On the ground state of the titanium phospide, TiP. A theoretical investigation", D. Tzeli and A. Mavridis, *J. Chem. Phys.* **121**, 2646 (2004). [DOI: 10.1063/1.1768159]

12. "The dipole moments of the excited states of FeC", D. Tzeli and A. Mavridis, *J. Chem. Phys.* **122**, 056101 (2005). [DOI: 10.1063/1.1834564]

13. "The CH ($X^2\Pi$, $a^4\Sigma^-$)...OH_2 and CH_2 (X^3B_1, a^1A_1)...OH_2 interactions. A first principles investigation" D. Tzeli and A. Mavridis, *Inter. J. Quantum Chem.* **104**, 497 (2005). [DOI: 10.1002/qua.20637]

14. "Theoretical investigation of the iron carbide cation, FeC^+", D. Tzeli and A. Mavridis, *J. Phys. Chem. A* **109**, 9249 (2005). [DOI: 10.1021/jp040765j]

15. "Ab initio Investigation of the Electronic and Geometric Structure of Magnesium Diboride, MgB_2", D. Tzeli and A. Mavridis, *J. Phys. Chem. A* **109** 10663 (2005). [DOI: 10.1021/jp058172b]

16. "The electronic structure of cobalt carbide, CoC", D. Tzeli and A. Mavridis, *J. Phys. Chem. A* **110**, 8952 (2006). [DOI: 10.1021/jp062357g]

17. "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] [Supporting information]

18. "Theoretical investigation of the ground and low-lying excited states of Nickel Carbide, NiC", D. Tzeli and A. Mavridis, *J. Chem. Phys.* **126**, 194304 (2007). [DOI: 10.1063/1.2723114]

19. "Theoretical study of adsorption of gallium and gallium nitrides on Si(111)", D. Tzeli, I. D. Petsalakis, G. Theodorakopoulos, *Chem. Phys. Lett.* 448, 88 (2007). [DOI: 10.1016/j.cplett.2007.09.060]

20. "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]

21. "The electron affinity of 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]

22. "Structure and energetics of InN and GaN dimers", L. Simova, D. Tzeli, M. Urban, I. Cernusak, G. Theodorakopoulos, I. Petsalakis, *Chem. Phys.* **349**, 98 (2008). [DOI: 10.1016/j.chemphys.2008.02.051]

23. "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] [Supplementary information intro, Supplementary information]

24. "Theoretical Study of Gallium Nitride Molecules, GaN_2 and GaN_4", D. Tzeli, G. Theodorakopoulos, and I. D. Petsalakis, *J. Phys. Chem. A* **112**, 8858 (2008) [DOI: 10.1021/jp8019396]

25. "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]

26. "Theoretical study of adsorption of group IIIA nitrides on Si(111)", D. Tzeli, I. Petsalakis, G. Theodorakopoulos, *J. Phys. Chem. C* **113**, 5563 (2009). [DOI: 10.1021/jp810838s]

27. "Theoretical study of adsorption and diffusion of group IIIA metals on Si(111)", D. Tzeli, I. Petsalakis, G. Theodorakopoulos, *J. Phys. Chem. C* **113**, 13924 (2009). [DOI: 10.1021/jp903389r] [Supporting information]

28. "Theoretical investigation of the ground and low-lying excited states of gallium and indium silicides, GaSi and InSi", D. Tzeli, I. D. Petsalakis, and G. Theodorakopoulos, *J. Chem. Phys.* **131**, 234301 (2009). [DOI: 10.1063/1.3271244]

29. "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]

30. "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]

31. "Theoretical investigation of the complexation of crown ethers and crown ethers of fulleropyrrolidine with $(CH_3)NH_{4-x}^+$, x = 0-4", D. Tzeli, I. Petsalakis, G. Theodorakopoulos, *Phys. Chem. Chem. Phys.* **13**, 954 (2011). [DOI: 10.1039/C0CP00180E]

32. "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, I. S. K. Kerkines and G. Theodorakopoulos, *Comp. Theor. Chem.* **965**, 168 (2011). [DOI: http://dx.doi.org/10.1016/j.comptc.2011.01.041] [Supplementary Material]

B. PAPERS IN REFEREED PROCEEDINGS OF INTERNATIONAL CONFERENCES

33. "A DFT Study of Adsorption of Gallium and Gallium Nitrides on Si(111)", D. Tzeli, G. Theodorakopoulos, and I. D. Petsalakis, in Frontiers in Quantum Systems in Chemistry

and Physics QSCP-XII, London 2007; S. Wilson et al. (eds.) [*Progr. Theor. Chem. Phys.* **18**] 341-350 (2008). [DOI: 10.1007/978-1-4020-8707-3_15]

34. "A theoretical study of complexes of crown ethers with substituted ammonium cations", D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, Progress in Theoretical Chemistry and Physics book of proceedings of the QSCP XV, in press (2011)