

CV of Dr. Demeter Tzeli

Date of birth: 05/02/1974
Marital Status: Married with five children
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12/7/1995: B.S. in Chemistry, Department of Chemistry, National and Kapodistrian University of Athens (NKUA), Greece
01/10/1997: M.Sc. in Physical Chemistry, Laboratory of Physical Chemistry, Department of Chemistry, NKUA, Greece
27/11/2000: Ph.D. in Quantum Chemistry, Laboratory of Physical Chemistry, Department of Chemistry, NKUA, Greece
12/2000-8/2006: Research Associate, Laboratory of Physical Chemistry, Department of Chemistry, NKUA, Greece.
12/2001-10/2002: Teacher of computer science in private college, KORELplus, 85 Akadimias, 10678 Athens, Greece.
9/2006-: Research Associate, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens 116 35, Greece.

• Honors and Awards

- Undergraduate:
 - Scholarship of Women Association of Trikala (for achieving the highest score at the entrance examinations for the Chemistry Department) 1991-1992.
 - National Scholarship Foundation of Greece (for academic achievement) 1991-1995.
- Graduate:
 - National Scholarship Foundation of Greece (11/1996-4/2000)
 - Associated Western Universities (AWU), USA, Laboratory Graduate Fellowship 27/7-4/9/1998.
- Post-doctoral:
 - Fellowship of Academy of Athens 9/2002-6/2004

• National, European and International Projects

- AWU program (7-9/1998)
“Studying the acetylene-water interaction, $C_2H_2-(H_2O)_n$, $n = 1 - 4$.”
PhD fellow, Pacific Northwest National Laboratory, Richland, U.S.A.
- SSATES, EPEAEK (5/1999-12/1999)
“Design and operation of station for continued upgrading of technological studies”
Teaching computer usage to undergraduate chemistry students at NKUA.
- Pythagoras, EPEAEK II (7/2004-8/2006)
This project is co-funded by the European Social Fund and National Resources.
“Accurate ab initio calculations on the $MC_x^{0,\pm 1}$, $MB_x^{0,\pm 1}$ M_y molecules, $M = Sc, Ti, V, Cr, Mn, Fe, Co, Ni$ and Cu , $x = 1, 2$, $y = 2, 3$.”
Researcher, Lab. Physical Chemistry, Department of Chemistry, NKUA, Greece.

4. HPC- Europa Transnational Access programme (24/10-13/11/2004)
 “Analysis of the chemical bonding of the superconductor MgB₂.”
 Research Associate Visitor, Theoretical Chemistry, Materials Science Center, Rijksuniversiteit Groningen, the Netherlands.
5. Greek-Slovakian collaboration
 “Theoretical calculations on clusters of GaN and InN molecules and their interaction with Si(111) surface.”
 Research Associate, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Ave., Athens

- **Scientific interests**

1. Accurate ab initio calculations via MRCI and CCSD(T) methods on small molecules, i.e., diatomic and triatomic molecules including transition metals. (Calculations of excited molecular states and their potential energy curves or surfaces, prediction of the spectra, calculation of the relativistic effects, etc).
2. Study of van der Waals systems, interactions of water with “hydrophobic” organic molecules via MP and CC methods.
3. Study of large systems such as solid state and interactions of small molecules with surfaces mostly via DFT methods.

- **Publications**

1. On the electronic structure of ground ($X^3\Sigma^-$) and some low-lying excited states ($A^3\Pi$, $a^1\Delta$, $b^1\Sigma^+$ and $B^3\Sigma^-$) of the isovalent species P-Li and P-Na.
 D. Tzeli, A. Papakondylis and A. Mavridis, *J. Mol. Struct. (THEOCHEM)*, **417**, 277-287 (1997).
2. On the electronic structure of NLi₂ and PLi₂ Ground and Low-Lying excited states.
 D. Tzeli, A. Papakondylis and A. Mavridis, *J. Phys. Chem. A* **102**, 2223-2230 (1998).
3. The electronic structure of ScAl⁺. Ground and Low-Lying excited states.
 D. Tzeli and A. Mavridis, *J. Phys. Chem. A* **104**, 6861-6870 (2000).
4. A first principles study of the acetylene-water interaction.
 D.Tzeli, A. Mavridis and S. Xantheas, *J. Chem. Phys.* **112**, 6178-6189 (2000).
5. First principles investigation of Boron and Aluminum Carbides, BC, AlC and their Anions, BC⁻ and AlC⁻. I
 D.Tzeli and A. Mavridis, *J. Phys. Chem. A* **105**, 1175-1184 (2001).
6. Accurate Theoretical Study of the Excited States of Boron and Aluminum Carbides, BC, AlC. II.
 D. Tzeli and A. Mavridis, *J. Phys. Chem. A* **105**, 7672-7685 (2001).
7. A molecular level study of the aqueous microsolvation of acetylene.
 D.Tzeli, A. Mavridis and S. Xantheas, *Chem. Phys. Lett.* **340**, 538-546 (2001).
8. Theoretical investigation of iron carbide, FeC.
 D. Tzeli and A. Mavridis, *J. Chem. Phys.* **116**, 4901-4921 (2002).
9. First Principles Examination of the Acetylene–Water clusters, HCCH–(H₂O)_x x = 2, 3, and 4.
 D.Tzeli, A. Mavridis and S. Xantheas, *J. Phys. Chem. A* **106**, 11327-11337 (2002).

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** 4984-4986 (2003).
11. On the ground state of titanium phosphide, TiP: A theoretical investigation.
D. Tzeli and A. Mavridis, *J. Chem. Phys.* **121**, 2646-2648 (2004).
12. The dipole moments of the excited states of FeC.
D. Tzeli and A. Mavridis, *J. Chem. Phys.* **122**, 056101-2 (2005).
13. The $CH(X^2\Pi, a^4\Sigma^-)\dots OH_2$ and $CH_2(\tilde{X}^3B_1, \tilde{a}^1A_1)\dots OH_2$ interactions.
A first principles investigation.
D. Tzeli and A. Mavridis, *Int. J. Quantum Chemistry* **104**, 497-511 (2005).
14. First principles investigation of the electronic structure of the iron carbide cation, FeC^+ .
D. Tzeli and A. Mavridis, *J. Phys. Chem. A* **109**, 9249-9258 (2005).
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**, 10663-10674 (2005).
16. Electronic structure of cobalt carbide, CoC.
D. Tzeli and A. Mavridis, *J. Phys. Chem. A* **110**, 8952-8962 (2006).
17. Theoretical investigation of the ground and low-lying excited states of Nickel Carbide, NiC.
D. Tzeli and A. Mavridis, *J. Chem. Phys.* **126**, 19304(1-12), (2007).
18. 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**, 8892-8902 (2007).
19. Theoretical study of adsorption of gallium and gallium nitrides on Si(111).
D. Tzeli, I. D. Petsalakis and G. Theodorakopoulos, *Chem. Phys. Lett.* **448**, 88-92 (2007).
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(1-14) (2008).
21. A DFT study of adsorption of gallium and gallium nitrides on Si(111).
D. Tzeli, G. Theodorakopoulos, and I. D. Petsalakis (Proceedings of the QCSP-XII, Frontiers in Quantum Systems in Chemistry and Physics – PTCP, **18**, xxx (2008)
22. Structure and Energetics of InN and GaN Dimers.
Lucia Šimová, Demeter Tzeli, Miroslav Urban, Ivan Černušák, G. Theodorakopoulos, and I. Petsalakis *Chem. Phys.* **xxx**, xxx (2008) Lischka's Special Issue.
23. The electron affinity of the gallium nitride (GaN) and digallium nitride (GaN₂). The importance of the basis set superposition error in strongly bound systems.
D. Tzeli and A. A. Tsekouras, *J. Chem. Phys.* **128**, 144103(1-7) (2008).
24. Theoretical study of the Gallium Nitride molecules, GaN_2 and GaN_4 .
D. Tzeli, G. Theodorakopoulos and I. D. Petsalakis *J. Phys. Chem. A*, accepted (2008)

- **Conferences**

1. *NATO ASI, "Recent Theoretical and Experimental Advances in Hydrogen-Bonded Clusters"*
Elounda, Crete, Greece, 22/6-4/7/1997.
2. *NATO ASI, "Quantum Monte Carlo in Physics and Chemistry"*
Summer School, Cornell University, Ithaca, N.Y., 13-24/7/1998.

3. *NATO ASI, "Metal-Ligand Interactions in Chemistry Physics and Biology"*
Cetrano (CS), Calabria, Italy, 1-12/9/1998.
4. *Fourth European Workshop on Quantum Systems in Chemistry and Physics,*
Marly-le-Roi, Paris, France, 22-27/4/1999.
5. *23rd International Workshop on Condensed Matter Theories,*
Ithaca, Greece, 17-23/6/1999.
6. *Fifth European Workshop on Quantum Systems in Chemistry and Physics,*
Uppsala University, Sweden, 13-18/4/2000.
7. *Sixth European Workshop on Quantum Systems in Chemistry and Physics,*
Sofia, Bulgaria, 19-24/4/2001.
8. *Eighth European Workshop on Quantum Systems in Chemistry and Physics,*
Spetses, Greece, 30/8 – 4/9/2003.
9. *Molecular Quantum Mechanics: The No Nonsense Path to Progress*
International Conference in honour of Nicholas C. Handy
St. John's College, Cambridge University, England, 24 – 29/7/2004.
10. *Quantum Systems in Chemistry and Physics, Workshop, QSCP XII*
Royal Holloway, University of London, U.K., 30/8 – 5/9/2007.