

## 1- MU\_FSCI\_CHEM\_INOR\_DATA\_Ahmed.El-Nahas



**Name\_:** Ahmed Mahmoud El-Nahas

**Date and place of birth:** 28-11-1964, El-Menoufia, Egypt

**Permanent address:** Chemistry Department, Faculty of Science, El-Menoufia University, Shebin El-Kom, Egypt

**Email:** [amelnahas@hotmail.com](mailto:amelnahas@hotmail.com)

**Tel:** 002-048-2239-756 (home), **mobile:** 002-016-4607974, **Fax:** 002-048-2235-689

**Family Status:** Married with two sons

### **Education:**

B.Sc. in chemistry, May 1986, faculty of Science, El-Menoufia University

M.Sc. in inorganic chemistry, Feb. 1990, faculty of science, El-Menoufia University

The M.Sc. entitled " MNDO Study of VSEPR Model Applied to 'N' Electron Pair Systems "

Ph.D. in inorganic chemistry, Oct. 1993, faculty of science, El-Menoufia University,

The Ph. D. was accomplished at Erlangen-Nuernberg University, Germany under supervision of Prof. P.v.R. Schleyer and the degree was awarded in Egypt. The Ph.D. thesis entitled " Structural Studies of Main Group Molecules " in this project we used Ab initio MO calculations with Gaussain 90 and 92 suits of programs.

### **Occupations:**

March 1988- Jan. 1990 *Demonstrator* in chemistry, Faculty of Science, El-Menoufia University, Shebin El-Kom, Egypt.

Feb. 1990-Oct. 1993 *Assistant Lecturer* in inorganic chemistry, faculty of science, El-Menoufia University, Shebin El-Kom, Egypt.

Nov. 1993-Nov. 1999: *Lecturer* of inorganic chemistry, faculty of science, El-Menoufia University, Shebin El-Kom, Egypt.

Dec. 1999-May 2005: *Associate professor* of physical chemistry, Faculty of Science, El-Menoufia University, Shebin El-Kom, Egypt.

June 2005-until now: *Professor* of physical chemistry, Faculty of Science, El-Menoufia University, Shebin El-Kom, Egypt.

**Main field:**

Computational Chemistry

**Points of interest:**

Existence of multiply charged systems, Atmospheric and Combustion Chemistry, Stabilities and structures of organic compounds, Conformational analysis, Tautomerism, Hydrogen bond strength, Reaction mechanism, Metal complexes, Stability of highly reactive group 14 containing compounds, Adsorption of metal ions and organic compounds over surfaces, and drug design.

Experiences:

**1. Software (MOPAC, GAUSSIAN, GAMESS, POLYRATE, and GAUSSRATE).**

2. Teaching of principles of quantum and physical chemistry for undergraduate level and quantum chemistry and group theory at the postgraduate level.

3. Participating in 12 conferences, in Egypt (4), Greece (1), England (1), Sweden (1), and Japan (5).

4. About 39 papers in quantum chemical applications in chemistry.

**Languages:**

Arabic (Native), English (very good), German (fair), Japanese (poor).

**2- MU\_FSCI\_CHEM\_INOR\_LINK\_Ahmed.El-Nahas**

**Email:** [amelnahas@hotmail.com](mailto:amelnahas@hotmail.com)

**Fellowships:**

**1/7/1991-1/7/1993:** A Ph.D. grant from the Egyptian government to Institute for Organic Chemistry, Erlangen-Nuernberg University, Germany with Prof. P.v.R. Schleyer

**1/3/1995-1/6/1995:** A grant from El-Menoufia University to the Computer Chemistry Centre/Institute of Organic Chemistry, Erlangen-Nuernberg University, Germany with Prof. p.v.R.Schleyer and Dr. T. Clark

**7/11/1997-6/11/1999:** *JSPS* postdoctoral fellowship (Japanese Society for the Promotion of Science) to Department of Applied Chemistry, School of Engineering, University of Tokyo, Japan with Prof. K. Hirao

**March 2002-Jan 2003** Postdoc at the Department of Organic Chemistry, Institute of Chemistry, Uppsala University, Sweden with Prof. Henrik Ottosson.

**December 2003-March 2005** Postdoc at Advanced Institute of Science and Technology (AIST), Tsukuba, Japan with Prof. Tadafumi Uchimaru

**September 2005-August 2007** Experienced researcher at Environmental Change Institute (ECI), the National University of Ireland, Galway (NUIG) with Prof. John Simmie

## Publications list for Professor Ahmed M. El-Nahas

1. Ahmed M. El-Nahas and P. v. R. Schleyer, Structures and Stabilization Energies of Methyl Anions with Main Group Substituents from the First Five Period, *J. Comput. Chem.* 15, 596-626 (1994).
2. Ahmed M. El-Nahas and T. Clark, AM1 and PM3 Calculations on the Effect of Substituents on the Stabilities of Carbocations in the Gas Phase and in Solution, *J. Org. Chem.* 60, 8023-8027 (1995).
3. J. Kapp, C. Schade, A. El-Nahas and P. v. R. Schleyer, Heavy Element Lone Pair Donors are not Less Effective, *J. Angew. Chem. Int. Ed. Engl.* 2236-2238 (1996).
4. Ahmed M. El-Nahas, Carbanion Stability: A Semiempirical AM1 and PM3 Study in the Gas Phase and in Solution, *J. Chem. Res. (S)* 310-311; (M) 1701-1715 (1996).
5. A. S. Shalabi and Ahmed M. El-Nahas, Bond functions and many-body effects of the helium Trimer, *Theor. Chem. Acc.* 96, 217-222 (1997).
6. Ahmed M. El-Nahas, Semiempirical and Ab Initio Calculations of Tautomerism in 2,3-Dihydroxypyrazine, *J. Chem. Res. (S)* 222-223; (M) 1014-1031 (1998).
7. Ahmed M. El-Nahas, E. Hammam and E.-Z.y M. Ebeid, Quantum Chemical Studies on Structures and Spectra of 2,5-Distyrylpyrazine (DSP) Laser Dye, *J. Comput. Chem.* 19, 585-592 (1998).
8. E. Hammam and Ahmed M. El-Nahas, Theoretical Study on Photophysical and Photochemical Properties of a Merocyanine Dye, *J. Phys. Chem. A* 102, 9739-9744 (1998).
9. Ahmed M. El-Nahas and K. Hirao, A theoretical study on 2-hydroxypyrazine and 2,3-dihydroxypyrazine: tautomerism, intramolecular hydrogen bond, solvent effect, *J. Mol. Struct. (THEOCHEM)* 459, 229-237 (1999).
10. Ahmed M. El-Nahas, N. Tajima and K. Hirao, Binding energies and electronic structures of  $\text{Cu}^+(\text{OH})_n$  and  $\text{Cu}^+(\text{NH}_3)_n$  ( $n=1-4$ ): anomaly of the two ligand  $\text{Cu}^+$  complexes, *J. Mol. Struct. (THEOCHEM)* 469, 201-213 (1999).

11. N. Tajima, M. Hashimoto, F. Toyama, Ahmed M. El-Nahas and K. Hirao, A theoretical study on the catalysis of Cu-exchanged zeolite for the decomposition of nitric oxide, *Phys. Chem. Chem. Phys.* 1, 3823-3830 (1999).
12. A. S. Shalabi, Ahmed M. El-Nahas, and A. A. Shalabi, Be<sup>2+</sup> V-Dipole and Adsorptivity of Atomic H on LiH(001) Surface: ab initio Study, *J. Mol. Mod.* 6, 26- 34 (2000).
13. Ahmed M. El-Nahas and K. Hirao, Complexation of Li<sup>+</sup> and Cu<sup>+</sup> with HX (X=F, Cl, OH, SH, NH<sub>2</sub>, and PH<sub>2</sub>) Molecules by B3LYP and CCSD(T) Methods, *J. Phys. Chem. A* 104, 138-144 (2000).
14. Ahmed M. El-Nahas, N. Tajima and K. Hirao, Do Cu<sup>2+</sup>+NH<sub>3</sub> and Cu<sup>2+</sup>+OH<sub>2</sub> exist?: Theory confirms 'yes!', *Chem. Phys. Lett.* 318, 333-339 (2000).
15. Ahmed M. El-Nahas, On the existence of Cu<sup>2+</sup>(NH<sub>3</sub>)<sub>1,2</sub> and Cu<sup>2+</sup>(OH<sub>2</sub>)<sub>1,2</sub> in the gas phase, *Chem. Phys. Lett.* 329, 176-178 (2000).
16. M. J. Mphahlele, M. A. Fernande, Ahmed M. El-Nahas, H. Ottosson, S. M. Ndlovu, H. M. Stithole, B. S. Dladla and D. De Waal, Solution phase, solid state and computational structural studies of the 2-aryl-3-bromo-quinolin-4(1H)-one derivatives, *J. Chem. Soc. Perkin Trans. II* 2159-2164 (2002).
17. A. F. Jalhout and Ahmed M. El-Nahas, Quantum Chemical Predictions of structures and vibrational spectra of formaldehyde and related molecules, *J. Mol. Struct. (THEOCHEM)* 671, 125-132 (2004).
18. A. M. El-Nahas, Thermochemically Stable M<sup>2+</sup>+OH<sub>2</sub> Complexes in the Gas Phase: M=Mn, Fe, Co, Ni, and Cu, *Chem. Phys. Lett.* 345, 325-330 (2001).
19. Ahmed M. El-Nahas, Monohydrated alkaline earth metal dications do exist, *Chem. Phys. Lett.* 348, 483-490 (2001).
20. Ahmed M. El-Nahas, Quantum chemical calculations on metal dications solvated by formaldehyde, acetone and DMSO ligands, *Chem. Phys. Lett.* 365, 251-259 (2002).
21. Ahmed M. El-Nahas, M. Johansson and H. Ottosson, Reverse Si=C Bond Polarization as a Means for Stabilization of Silabenzenes: A Computational Investigation, *Organometallic* 22, 5556-5566 (2003).

22. C. Xiao, F. Hagelberg and Ahmed M. El-Nahas, Density-Functional Study on the Structures, Stabilities and Dissociation Pathways of  $\text{Sc}^{3+}(\text{DMSO})_n$  Complexes ( $n=1-6$ ), *J. Phys. Chem. A* 108, 5322-5332 (2004).
23. Ahmed M. El-Nahas and M. J. Mphahlele, Conformational studies of potentially Tautomeric 2-phenyl- and 3-phenyl-1,4-benzoxazepin-5(4H)-one derivatives, *J. Mol. Struct. (THEOCHEM)* 668, 157-162 (2004).
24. C. Xiao, K. Walker, F. Hagelberg and Ahmed M. El-Nahas, Theoretical study on the structures and dissociation channels of metal dications solvated by acetonitrile ligands, *Int. J. Mass Spectrom.* 233, 87-98 (2004).
25. M. J. Mphahlele, Ahmed M. El-Nahas and T. El Gogary, Spectroscopic and quantum chemical studies of 2-arylquinoline-4(1H)-thione derivatives, *J. Mol. Struct.* 690, 151-157 (2004).
26. M. J. Mphahlele and Ahmed M. El-Nahas, Tautomeric 2-arylquinolin-4(1H)-one derivatives- spectroscopic, X-ray and quantum chemical structural studies, *J. Mol. Struct.* 688, 129-136 (2004).
27. Ahmed M. El-Nahas, C. Xiao and F. Hagelberg, Formation and unimolecular dissociation of  $\text{Al}^{3+}(\text{DMSO})_n$  complexes, *Int. J. Mass Spectrom.* 237, 47-54 (2004).
28. A. Jarid, S. Chafiq, Ahmed M. El-Nahas, H. Anane and M. Esseffar, Theoretical study of  $\text{H}_3\text{AXH}_3$  and  $\text{H}_3\text{AYH}_2$  ( $\text{A}=\text{B}$ , Al, Ga;  $\text{X}=\text{N}$ , P, As and  $\text{Y}=\text{O}$ , S, and Se), electrostatic and hyperconjugative interactions roles. Abdelaâli El Guerraze, *Chem. Phys.* 313, 159-168 (2005).
29. Ahmed M. El-Nahas, T. Uchimaru, M. Sugie, K. Tokuhashi and A. Sekiya, Hydrogen abstraction from dimethyl ether (DME) and dimethyl sulfide (DMS) by OH radical: A computational study, *J. Mol. Struct. (THEOCHEM)* 722, 9-19 (2005).
30. Ahmed M. El-Nahas, T. Uchimaru, M. Sugie, K. Tokuhashi and A. Sekiya, A Relative reactivity and regioselectivity of halogen-substituted ethenes and propene toward addition of an OH radical or O ( $^3\text{P}$ ) atom: An ab initio study, *J. Mol. Struct. (THEOCHEM)* 770 (2006) 59-65.
31. Ahmed M. El-Nahas, Joseph W. Bozzelli, John M. Simmie, Maria V. Navarro, Gráinne Black, and Henry J. Curran, Thermochemistry of

Acetonyl and Related Radicals, *J. Phys. Chem. A*. 110 (2006) 13618-13623.

32. Asem A. Atia, Ahmed M. El-Nahas, Laila D. AlMahdy, and Asmaa Marie, Adsorption of Oleic Acid on Silica Gel Derived from Rice Ash Hulls: Experimental and Theoretical Studies, *Adsorption Science and Technology*, 24 (2006) 797-814.

33. Ahmed M. El-Nahas, Maria V. Navarro, John M. Simmie, Joseph W. Bozzelli, Henry J. Curran, Wayne Metcalfe and Stephen Dooley, Enthalpies of Formation, Bond Dissociation Energies and Reaction Paths for the Decomposition of Model Biofuels: Methyl Butanoate and Ethyl Propanoate, *J. Phys. Chem. A* 111 (2007) 3727-3739.

34. Wayne K. Metcalfe, Stephen Dooley, Henry J. Curran, John M. Simmie, Ahmed M. El-Nahas, and Maria V. Navarro, Experimental and modeling Study of C<sub>5</sub>H<sub>10</sub>O<sub>2</sub> Ethyl and Methyl Esters, *J. Phys. Chem. A* 111 (2007) 4001-4014.

35. T. Uchimaru, Ahmed M. El-Nahas, M. Sugie, K. Tokuhashi and A. Sekiya, DFT/ab initio study on the reaction paths for the reaction of CH<sub>3</sub>SH with NO<sub>3</sub>, *Chem. Lett.* 36 (2007), 400-401.

36. Ahmed M. El-Nahas, Safinaz H. El-Demerdash, ElSayed E. El-Shereefy, Quantum Chemical Calculations on the Structure and Stability of Mg<sup>2+</sup>XH<sub>3</sub>OH Complexes in the Gas Phase (X=C, Si, and Ge), *International Journal of Mass Spectrometry* 263 (2007) 267-275.

37- Abraham F. Jalbout, B. Trzaskowski, Y. Xia, Y. Li, X. Hu, H. Li, Ahmed M. El-Nahas and Ludwik Adamowicz, Structures, stabilities and tautomerizations of uracil and diphosphouracil tautomers, *Chemical Physics* 332(2-3) (2007) 152-161.

38- Tarek M El-Gogary and Ahmed M. El-Nahas, Origin of reverse stability of diphosphouracil tautomers compared to their analogue uracil: DFT and Ab initio stud, *J. Molwec. Struct. (THEOCHEM)* 852 (2008) 54-62 .

39. Ahmed M. El-Nahas, John M. Simmie, Maria V. Navarro, Joseph W. Bozzelli, Gráinne Black, and Henry J. Curran, Mechanism and Kinetics of Acetonyl Radical Oxidation: A Quantum Chemistry and CVT/SCT Approach, *Phys. Chem. Chem. Phys.*, submitted.



40. Tahani .I. Kashar, Ahmed M El-Nahas, and Asmaa M. El-Mughamsi, Synthesis and Characterization of Mn(II), Fe(III), Co(II), Ni(II), Cu(II) and Zn(II) Complexes of PAAEH, Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, submitted.

41. Effect of structural properties of acidic dyes on their adsorption behaviour from aqueous solutions by amine modified silica, A. M. Donia, A. A. Atia, W. A. Al-amrani and Ahmed M. El-Nahas, Journal of Hazardous Materials, Submitted.