Nom : KOMIHA

Prénom :Najia

Date de naissance : le 9 Juin 1956

Nationalité : Marocaine

Adresse : Laboratoire de chimie théorique .Faculté des Sciences .Rabat Maroc.

Tel : (212) 37 77 54 40 Email : komiha@fsr.ac.ma

GSM :06 6190 93 77

EDUCATIONAL BACKGROUND AND DIPLOMAS

- French Baccalauréat série C of Bordeaux University obtained at Marrakech(1974).
- Licence in Chemistry University Mohammed V-Agdal Rabat-1978
- PHD University Paris VI – 1981 'Potential Energy surfaces of $N2O^+$, a radical ion concerned in atmospheric pollution '
- Doctorat d'état in Physical Chemistry at University Mohammed V-Agdal Rabat - 1986 in collaborationwith University of Paul Sabatier Toulouse France intitled :

' Theoretical study of negative ions of astrophysical interest'.

***PROFESSIONAL EXPERIENCE*:**

Recruited as assistant professor in 1981 at the Faculty of Science of Rabat..

1981-1986 : assistant Professor

1986- : Full Professor

2011 : Vice Dean for research and cooperation of the faculty.

TEACHING :

Pratical works in general, organic and physical chemistry at bachelor, master and PHD level .

Theoretical quantum chemistry at Bachelor, Master and PHD level.

Lessons and courses published on the web site of our institution.

PARTICIPATION TO THE DEPARTEMENT ACTIVITIES:

Head of the teoretical Chemistry Lab since 1999.

Member of the department college for two terms.

Responsibility of the library: purchases of books, documents, computers.
Organization of conferences, workshops and missions.

Acquisition for the theoretical chemistry lab of equipment and molecular calculations programs.

Member of the committee responsible for the computerization of the faculty
Founding member of the Moroccan Association for theoretical chemists (AMCT), Vice president of that association

RESEARCH ACTIVITIES :

- Active member of the Laboratory of Theoretical Chemistry since 1981. Head of the Laboratory of Theoretical Chemistry in Rabat since 1999.
- Vice Dean for research and cooperation since 2012.
- Research interest : environment , atmospheric pollution, astrophysics and reactivity for new molecules invention.

The methods of quantum chemistry used to study these problems are of several types:

The semi-empirical methods: CNDO,MNDO,AM1,PM3,EHT ;

Ab-initio methods : Hartree-Fock and post Hartree-Fock calculations;configuration interaction approaches,Density Functional méthods (DFT) and Coupled Cluster methods .

PUBLICATIONS:

2015:

41) 'Article: Ab-initio potential energy curves of valence and Rydberg electronic states of the PO radical'

S.Izzaouiha, H.Abou El Makarim, N.Komiha*,S.Lahmar,H.Ghalila

Journal of Computational and Theoretical Chemistry(accepted)

2014:

40) ' Ab initio study of PN electronic states–a qualitative interpretation of the perturbation and predissociation effects on observed transitions'

K.Abbiche, M.Salah, K.Marachi, O.K.Kabbaj, N.Komiha

Molecular Physics, 2014 Vol. 112, No. 1, 117–126

39) ' DFT study of the mechanism and stereoselectivity of the 1,3-dipolar

cycloaddition between pyrroline-1-oxide and methyl crotonate

Khadija Marakchi, Rachida Ghailane, Oum Kaltoum Kabbaj and

Najia Komiha

J. Chem. Sci. Vol. 126, No. 1, January 2014, pp. 283–292. Indian Academy of Sciences.

38) Accurate theoretical spectroscopy of the lowest electronic states of CP radical

Abbiche, K., Marakchi, K., Komiha, N., Francisco, J.S., Linguerri, R., Hochlaf, M.

Molecular Physics 2014

2013:

37) 'Experimental and theoretical studies for mild steel corrosion inhibition in 1 M HCl

by two new benzothiazine derivatives '

R.Ghailane, K.Marakchi, A.Souizi, T.Ghailane,N.Komiha

Corrosion Science Volume: 76 Pages: 317-324

2012:

36) 'Solvation effects and stabilization of multicharged ions: a case study of Arm BeOq+ complexes'

M.Hochlaf, R.Linguerri, N.Komiha. Physical Chemistry Chemical Physics Volume: 14 Issue: 12 Pages: 4236-4243 DOI: 10.1039/c2cp24004a Published: 2012

35) 'Molecular structure and vibrational study of diprotonated guanazolium using DFT calculations and FT-IR and FT-Raman spectroscopies

Guennoun, L ; Zaydoun, S ; El Jastimi; Marakchi, K ; Komiha, N ; Kabbaj, OK ; El

Hajji, A ; Guedira, F

Spectrochimica Acta Part A-Molecular And Biomolecular Spectroscopy Volume: 97

Pages: 975-985

2011 :

34) 'Modélisation et simulation quantiques en chimie : une expérience Marocaine' Actes de la session plénière de l'Académie Hassan II des Sciences et Techniques. 215-225,Mars 2011.

2010:

33) ' Theoretical Study Of The Mechanism Of The 1,3-Dipolar Cycloaddition Reaction of Methyl-3-Fluoro-3- Trifluoromethyl Prop-2-Enoate With Pyrroline-1-Oxide'

K. Marakchi, H. Abou El Makarim, O. K. Kabbaj, N. Komiha

Phys. Chem. News 52 (2010) 128-136

32) 'On the formation of S2O at low energies: an ab-initio study'

Isabelle Navizet, Najia Komiha, Roberto Linguerri, Gilberte Chambaud and Pavel Rosmus

Chemical Physics Letters, Volume 500, Issues 4-6, 19 November 2010, Pages 207-210

2009 **:**

31) 'Relationship Between Antioxidant Acidity of Several Flavonols And Their Molecular Properties'

E.H. Anouar, K. Marakchi, N. Komiha*, OK. Kabbaj, Z. Dhaouadi, S. Lahmar

Phys. Chem. News 45 (2009) 107-113 PCN 107

30) 'Erratum: Dipole moments and orientation polarizabilities of diatomic molecular ions for precision atomic mass measurement '

Michelle Cheng, John M. Brown, Pavel Rosmus, Roberto Linguerri, Najia Komiha, and Edmund G. Myers

Physical Review A 79, 059903(E) (2009),

2008 :

29) 'Electronic states of the Ultramarine chromophore S3-'

R.Linguerri,N.Komiha,J.Fabian,P.Rosmus

Z.Phys.chem.,222(1),2008,163-176

28) 'Electronic states of BP,BP+,BP-,B2P2, B2P2-and B2P2+'

R.Linguerri,N.Komiha,R.Oswald,A.Mitrushenkov,P.Rosmus

Chem.Phys. 346(2008) 1-7

27) Research Article 'First principle computations of rotational-vibrational transition probabilities'

P.Rosmus,R.Linguerri, N.Komiha

Molecular Physics 106(16-18) ,(2008),2001-2009

2007:

26) 'On the electronic states of S4+ and S4- isomers'

H.Sormova,R.Linguerri,P.Rosmus,J.Fabian,N.Komiha

Collect.Czech.Chem.Commun., Vol 72(1),2007,83-99.

25) 'Dipole Moments and Orientation Polarisabilities of Diatomic Molecular Ions for Precision Atomic Mass Measurement'

M.Cheng,J.M.Brown,P.Rosmus,R.Linguerri,N.Komiha, Phys.Rev.A 75,2007,12502(14)

24) 'Low lying quartet states in diacetylene,triacetylene and benzene radical cations'

N.Komiha,P.Rosmus;J.P.Maier, Mol.Phys.,Vol 105(5-7),2007,893-897.

23) 'Exploring QSAR of non-nucleoside reverse transcriptase inhibitors by artificial neural network :HEPT derivates'

M.Zahouily,J.Rakik,M.Lazar,M.A.Bahlaoui,A.Rayadh,N.Komiha

General Papers ARKIVOC (xiv)2007,245-256.

2006:

22) 'The spin-orbit coupling in the bond formation region of the electronic ground states of O3+,S3+ andSO2+ '

I.Navizet,G.Chambaud, P.Rosmus, N.Komiha

Chem.Phys.,329,issues 1-3,2006,251-259

21) 'Low lying quartet states in diacetylene,triacetylene and benzene radical cations'

N.Komiha,P.Rosmus;J.P.Maier, Mol.Phys.,Vol 104-20-21),2006,3281-3285.

20) 'The absorption wavelengths of sulphur chromophors of ultramarines calculated by time-dependant density functional theory'

J.Fabian,N.Komiha,R.Linguerri,P.Rosmus, J.of Mol.Struct.(THEOCHEM) , vol 801,issue 1-3,2006,63-69

2005:

19) 'A density functionnal study of htero-Diels-Alder reactions with substituted nitrosoalkenes'

N.KOMIHA,O.K.Kabbaj,S.Lafquih-Titouani, Internet Electronic J.of Mol.Design,2005,4,ISSN 1538

2003:

18) 'Ab initio and DFT studies on mechanism of the 1,3-dipolar cycloaddition reaction between nitrone and sulfonylethene chloride'

K.Marakchi, O.Kabbaj,N.Komiha,R.Jallal , M.Essefar.

J.Mol.Struct.(THEOCHEM) 2003,620 :2-3 :271-281 .

17)‘ A density functionnal study of Alizarin, two of its isomers and its transition metals and rare-earth complexes‘
N.Komiha,O.K.Kabbaj,M.Chraibi,J.Mol.Struct.(THEOCHEM) 2003,620 :2-3 :271-281

2001:

16) ‘ Theoritical study of the electronic attachement dissociation of the freon

molecules: CF3Cl , CF2Cl2 , CFCl3 ‘

N.Komiha , O.K.Kabbaj , M.Chraibi ,J.Fluorine .Chem. ,2001,108 2:177-186

15)’ Etude théorique des reactions de cycloaddition dipolaire-1,3 de la diphénylnitrilimine sur des dipolarophiles hautement fluorés’

K.Marakchi,O.K.Kabbaj,N.Komiha,M.L.Chraibi,J.Fluorine .Chem. ,2001,109,163-171.

14)’ Etude vibrationnelle et théorique de la protonation du 3,4’-bi-1,2,4-triazole et de ses derives C-bromé et C-méthylé.’

F.Guédira , N.Ouijja ,S.Zaydoun, N.Komiha,A.Lautié,M.Saidi-Idrissi

Canadian J. of An.Sc.and Spect.,2001, Vol 46(1).

2000:

13) ‘ A theoretical investigation of the conformational aspects of aminophenols and of

their complexation with BF2+ and ZnCl2 ‘
R.Ghailane,K.Marrakchi,N.Komiha,O.K.Kabbaj,M.Chraibi,N.Habbadi,M.Dartiguenav

J.Mol.Struct.(THEOCHEM) 2000,531 :1-3 :223-239 .

1995:

12) ‘ A representation of effective potentials of molecular fragments (NH3,PH3,AsH3) ..’ Z.Sekkat,N.Komiha,M.Chraibi, J.Mol.Struct.(THEOCHEM),1995 ,358,219-228

1994:

11) ‘ Ab-initio study of the predissociation processes of the ground and first excited states of N2O+.Potential curves of the lowest states of N2O+. ‘N.Komiha , J.Mol.Struct.(THEOCHEM),1994,306,313-320

10) ‘ Etude théorique de la prédissociation des premiers états excités de N2O- ..’ R.Ghailane,N.Komiha,M.Chraibi,J.Soc.Mar.Chim.,3,18,1994

1993 :

9) ‘Détermination d’un potentiel du groupe PH3 : test sur la molécule PH3-BH3 et sur les complexes (PH3)3Cu-BH4 ‘ H.Aboulmakarim,R.Ghailane,N.Komiha ,J.Mol.Struct.(THEOCHEM),1993,228,261-271

8) ‘Etude théorique de la dissociation de NO par attachement électronique ...’ R.Ghailane,N.Komiha,M.Chraibi , J.Mol.Struct.(THEOCHEM),1993,279,7-14

7) Etude Ab-initio SCF+IC des états spectroscopiques et de l’affinité electronique de B ,C ,N et F..’ A.ElKaroini, R.Ghailane, S.Jorio,N.Komiha,O.K.Kabbaj,M.Chraibi , J.Mol.Struct.(THEOCHEM),1993,279,1-6

1992 :

6) ‘Etude théorique de la dissociation de CO par attachement électronique ..’ , A.ElKaroini, R.Ghailane,N.Komiha,M.Chraibi,J.Soc.Mar.Chim.1,49_57,1992

1991:

5) ‘Etude théorique des spectres photoélectroniques et ultraviolet de l’anion CN-‘ N.Komiha , M.Chraibi ,Journal of Molecular structure (THEOCHEM) 1991, 228,11-17

4) ‘ Etude ab-initio des états excités de OH-‘,N.Komiha,A.Elkaroini,M.Hliwa, J.Mol.Struct.(THEOCHEM),1991,251,29-36

1987:

3) ‘Diabatic research of resonnant states in MO-CI calculations of négative ions ‘ N.Komiha,J.P.Daudey,J.P.Malrieu,J.Phys.B :At.Mol.Phys.,1987,20,4375-4391

1988:

2) ‘One-Center expansion for pseudopotential Matrix elements ‘ M.Pelissier , N.Komiha , J.P.Daudey,Journal of Comp.Chem. 1988,vol 9,4,298-302

1985:

1) ‘ On stability of cubic P8 ‘ G.Trinquier , J.P.Daudey, N.Komiha, Journal of american chemical society , 1985 ,107,7210-7212

Conferences and workshop Organisations

4th school of quantum chemistry-Faculty of Sciences-Rabat-June 2014

National Science Weeks- Faculty of Sciences-Rabat- 2012,2013,2014

'The Doctoriales'-Faculty of Sciences-Rabat- 2013,2014

3rd school of quantum chemistry-Rabat-June 2009

2nd school of Theoretical and modelling chemistry, Fès April 2008.

2nd National meeting of the theoretical chemists ENACT, Errachidia 2007.

3rd National Meeting of theoretical Chemistry, Kénitra 2006.

1st International Congres of Modélisation Moléculaire, Casablanca 2005.

1st summer school of molecular modelling PEMM, El Jadida 2004.

Meeting on theoretical chemistry teaching, Meknès 2003.

1rst National meeting of quantum chemists RENACT, Fès 2002.

COLLABORATIONS :

- Theoretical Chemistry labs of Fes , Marrakech ,Kénitra et Meknes .
- Laboratory MSME University of Marne La Vallée France
- Laboratory of Physique Quantique of University Paul Sabatier Toulouse. France
- Laboratory of spectroscopy of atomic and molecular systems –TUNIS.

RESEARCH CONVENTIONS :

- With the CNRST (Maroccan Center of Research and Technology) project for the study of molecules of economical interest PARS.
- With Tunisia (Laboratoire de spectroscopie de Tunis Manar). projet MT34-2006-2008
- Project ' plan d'urgence pour la recherche' SCH09/09-2009-2013
- Marocco-Tunisian project 12/TM 07(IPEST-La Marsa) 2012-2014
- Européen Project : Marie Curie: CO2 capture by Zéolithes.

European PF7 Marie Curie PIRSES-GA-2012-317544 project CapZeo . 2012-2016

Expertise:

- Vice Dean for Reseach and cooperation at the FSR 2011-
- Expert for evaluations of the scientific comittees of CNRST 2011-
- Membrer of editorial board de Mediteranean Journal of Chemistry
- Vice Présidente of the "Association Marocaine des Chimistes Théoriciens'.