

Xabier Lopez

Curriculum Vitae

Mailing Address

Dr. Xabier Lopez
Kimika Fakultatea
Euskal Herriko Unibertsitatea
P.K. 1072
20080 Donostia; Spain
tel: +34-943-018186
fax: +34-943-015270
e-mail: poplopex@sq.ehu.es

Personal Data

Date of Birth	Aug. 4, 1968
Place of Birth	Donostia, (Spain)
Nationality	Spanish
Marital Status	Married
Languages	Spanish (mother language), English (good). French (good), Basque (good).

Education

- [1991 - 1996] Graduate Education: *Doctorat* in Quantum Chemistry.
University of the Basque Country , Donostia , Spain.
Dissertation (in English): *On the Gas-Phase Chemistry of P⁺:
Ionic Clusters, Dioxides and Interstellar Chemistry.*
Grade:: *Apto Cum Laudem.*
Supervisor: Prof. Jesus M. Ugalde.
- [1986 - 1991] Undergraduate Education: Licenciature in Chemistry
Universidad Autonoma de Madrid, Madrid , Spain.

Experience

- [Nov 00 -] Associate Professor at the Department of Chemistry in the Univeristy of the Basque Count
- [Sept 99 -Oct 00] Postdoctoral Research Associate in the group of Prof. W. G. Richards
Oxford Centre for Molecular Science, New Chemistry Lab, Oxford (United Kingdom).
- [Jan 97 - Sept 99] Postdoctoral Research Associate under the supervision of
Prof. M. Karplus, Universite Louis Pasteur, Strasbourg (France).
- [Mar 96 - Nov 96] Research Associate with Prof. J.M. Ugalde
University of the Basque Country, Donostia, Spain

Fellowships and Contracts

- [Nov 00 -] Associate Professor at the University of the Basque Country San Sebastian, Spain
- [Jan 99 - Oct 00] *Marie-Curie Research Trainning Grant*
Postdoctoral fellowship to work with Prof. M. Karplus at the Universite Louis Pasteur Strasbourg, France.
- [Jan 97 - Dic 98] Postdoctoral Fellowship from the Spanish Education and Culture Office (M.E.C.) to work in the group of Prof. M. Karplus at the Universite Louis Pasteur, Strasbourg, France.
- [Mar 96 - Nov 96] Postdoctoral Fellowship from Basque Country University to work in the group of the Prof. J.M. Ugalde.
- [Oct 91 - Oct 95] Fellowship of the Government of the Basque Country for doctoral studies, under supervision del Prof. J.M. Ugalde

Relevant Scientific Techniques and Skills Acquired

Operating Systems: UNIX, MS-DOS, LINUX

Programation : C, Fortran, awk, Perl

Programs used: CHARMM, GAUSSIAN, GAMESS, CADPACK, UHBD, MOPAC, AIMPAC

Tools : MOLMOL, MOLDEN, EXCEL

Publication List

1. F.P. Cossio, J.M. Ugalde, X. Lopez, B. Lecea and C. Palomo
A Semiempirical Theoretical Study of the Formation of β -Lactams from Ketenes and Imines
Journal of American Chemical Society, **115**, 995 - 1004 (1993).
2. X. Lopez, J.M. Ugalde, C. Barrientos, A. Largo and P. Redondo
Theoretical Study of Possible Processes for the Interstellar Production of Phosphorus Compounds. Reactions of P^+ with SH_2
Journal of Physical Chemistry, **97**, 1521 - 1525 (1993).
3. X. Lopez, C. Sarasola, B. Lecea, A. Largo, C. Barrientos and J.M. Ugalde
Ab-Initio Characterization of P_2O_2 Oxyde.
Journal of Physical Chemistry, **97**, 4078 - 4079 (1993).
4. C. Sarasola, X. Lopez, A. Arrieta, C. Barrientos, A. Largo and J.M. Ugalde
Ab Initio Characterization of Novel Gaseous $(PO)_2^+$ Compounds
Journal of Physical Chemistry, **97**, 5860 - 5863 (1993).
5. X. Lopez, J.M. Ugalde, F.P. Cossio, B. Lecea, A. Largo, C. Barrientos
Ab Initio Study of Phosphorus Ion Complexes of Ammonia and Water
Journal of Physical Chemistry, **97**, 9337 - 9340 (1993).
6. F.P. Cossio, B. Lecea, X. Lopez, G. Roa, A. Arrieta, J.M. Ugalde
An Ab Initio Study of the Mechanism of the Alkene-Isocyanate Cycloaddition to Form β -Lactams
Journal of Chemical Society Chemical Communications **18**, 1450 - 1452 (1993).
7. Leif. A. Eriksson, X. Lopez and Russell J. Boyd
On the Choice of the Active Space and the Basis Set for MCSCF Calculations on Small Molecules and Reactive Surfaces
Journal of Physical Chemistry, **97**, 11969 - 11973 (1993).
8. J. Maiz, A. Arrieta, X. Lopez, J.M. Ugalde, F.P. Cossio
Transition Structures for the Reformatsky Reaction. A Theoretical (MNDO-PM3) Study.
Tetrahedron Letters **34**, 6111 - 6114 (1993).
9. X. Lopez, F.P. Cossio, J.M. Ugalde, C. Barrientos and A. Largo.
Ab Initio Characterization of Gaseous $(CO_2P)^+$
Journal of Physical Chemistry, **98**, 2294 - 2297 (1994).

10. X. Lopez, J.M. Ugalde, F.P. Cossio, A. Largo and C. Barrientos
Topological Analysis of the Charge Density for Phosphorus Ion-Molecule Complexes Bound to Water and Ammonia Molecules
Journal of Physical Chemistry. **98**, 3148 - 3153 (1994).
11. A. Largo, C. Barrientos, X. Lopez and J.M. Ugalde
Theoretical Study of the C_2P Radical and $(C_2P)^+$ Species
Journal of Physical Chemistry, **98**, 3985 - 3988 (1994).
12. X. Lopez, A. Irigoras, J.M. Ugalde and F.P. Cossio
Characterization of the PL_n^+ Ion Molecule Clusters of the First and Second Row Hydrides
Journal of American Chemical Society, **116**, 10670 - 10678 (1994).
13. A. Largo, C. Barrientos, X. Lopez, F.P. Cossio and J.M. Ugalde
Theoretical Studies of Possible Processes for Interstellar Production of Phosphorus Compounds. The Reaction of P^+ with Acetylene.
Journal of Physical Chemistry, **99**, 6432 - 6440 (1995).
14. X. Lopez, M. Ayerbe, J.M. Ugalde, F.P. Cossio
Mechanisms for the Reaction of Triplet P^+ with XH ($X=3DCl,F$). Formation of the $P-X$ Bond.
Journal of Physical Chemistry, **99**, 6812 - 6818 (1995).
15. E.M. Cruz, X. Lopez, J.M. Ugalde and F.P. Cossio
G1 and G2 Study of the Triplet $[H_4, C, O, P]^+$ Potential Energy Surface. Mechanisms for the Reaction of P^+ (3P) with Methanol.
Journal of Physical Chemistry, **99**, 12170 - 12178 (1995).
16. B. Lecea, A. Arrieta, X. Lopez, J.M. Ugalde, F.P. Cossio. *On the Stereochemical Outcome of the Catalyzed and Uncatalyzed Cycloaddition Reaction Between Activated Ketenes and Aldehydes to Form cis and trans-2Oxetanones. An Ab-Initio Study*
Journal of American Chemical Society, **117** 12314 (1995).
17. X. Lopez, J.M. Ugalde and F.P. Cossio
Characterization of the $(P^+L_x)L_y$ Ion-Molecule Clusters of the First Row Hydrides
Journal of American Chemical Society, **118**, 2718 - 2725 (1996).
18. B.Lecea, I. Arrastia, A. Arrieta, G. Roa, X. Lopez, M.I. Arriortua, J.M. Ugalde and F.P. Cossio
Solvent and Substituent Effects in the Periselectivity of the Staudinger Reaction Between Ketenes and alpha,beta unsaturated imines. A Theoretical and Experimental Study.
Journal of Organic Chemistry, **61**, 3070 - 3079 (1996).

19. X. Lopez, J.M. Ugalde, C. Sarasola and F.P. Cossio
On the Accuracy of Density Functional Theory for Ion-Molecule Clusters. A Case Study of PL_n^+ Clusters of the First and Second Row Hydrides
Canadian Journal of Chemistry, **74**, 1032 - 1048 (1996).
20. A. Irigoras, J.M. Ugalde, X. Lopez and C. Sarasola
On the Dissociation Energy of $Ti(OH_2)^+$. An MCSCF and DFT Study.
Canadian Journal of Chemistry, **74**, 1824 - 1829 (1996).
21. X. Lopez, E.M. Cruz, M. Sarobe, J.M. Ugalde and F.P. Cossio
G1 and G2 Study of the Triplet $[H_4, Si, P]^+$ Potential Energy Surface. Reaction of P^+ (3P) with Silane.
Journal of Computational Chemistry, **18**, 9 - 19 (1997).
22. J.M. Ugalde, C. Sarasola and X. Lopez
Atomic and Molecular Bound Ground States of the Yukawa Potential.
Physical Review A., **56**, 1642 - 1645 (1997).
23. X. Lopez, C. Sarasola and J.M. Ugalde
Transition energies and emission oscillator strength of He in Model Plasma Environments.
Journal of Physical Chemistry A, **101**, 1804 - 1807 (1997).
24. E.M. Cruz, X. Lopez, M. Ayerbe, J.M. Ugalde
G2 study of the triplet and singlet $[H_3, P_2]^+$ potential energy surfaces. Mechanisms for the reaction of P^+ ($^3P, ^1D$) with PH_3 .
Journal of Physical Chemistry A., **101**, 2166 - 2172 (1997).
25. J.M. Mercero, X. Lopez, J.E. Fowler, J.M. Ugalde
Ab-initio studies of alternant X_2Y_2 rings ($X=^3D N, P, As, Sb; Y=^3D O, Se, Te$): planar versus butterfly species.
Journal of Physical Chemistry A, **101**, 5574 - 5579 (1997).
26. E.M. Cruz, J.E. Fowler, X. Lopez, J.M. Ugalde
The reaction of P^+ (3P) with methylamine: a detailed study of the potential energy surfaces and reaction mechanism.
Journal of Physical Chemistry A, **101**, 4807 - 4813 (1997).
27. X. Lopez, A. Dejaegere, M. Karplus
The Mechanism of Alkaline Hydrolysis of Cyclic and Acyclic Sulfates: An Ab-Initio Study with Solvation Correction
Journal of American Chemical Society. **121**, 5548 - 5559 (1999).
28. X. Lopez, A. Dejaegere and M. Karplus
Solvent Effects on the Reaction Coordinate of the Hydrolysis of Phosphates and Sulfates: Application of Hammond and Anti-Hammond Effects to Understand Hydrolysis in Solution
Journal of American Chemical Society, **123**, 11755 - 11763 (2001).

29. M. Schuman, X. Lopez, M. Karplus, Véronique Gouverneur.
Synthesis of a Novel Diarylphosphinic Acid: A Distorted Ground State Mimic and Transition State Analog for Amide Hydrolysis.
Tetrahedron, **57**, 10299-10307 (2001)
30. J.M. Mercero, A. Irigoras, X. Lopez, J.E. Fowler, J.M. Ugalde
Aluminum (III) Interactions with Sulfur containing Aminoacid chains.
Journal of Physical Chemistry A, **105**, 7446 - 7453 (2001).
31. X. Lopez, D.M. York, A. Dejaegere, M. Karplus
Theoretical Studies on the Hydrolysis of Phosphate diesters in the gas phase, solution and RNase A.
Int. J. of Quantum Chemistry, **86**, 10 - 26 (2002).
32. X. Lopez, M. Schaefer, A. Dejaegere, M. Karplus
Theoretical Evaluation of pK_a in Phosphoranes: Implications for Phosphate Ester Hydrolysis.
Journal of American Chemical Society, **124**, 5010 (2002).
33. J.M. Mercero, J.M. Matxain, X. Lopez, J.E. Fowler, J.M. Ugalde
Aluminum (III) Interactions with the side chains of aromatic aminoacids
International Journal of Quantum Chemistry, **90**, 90, 859 - 881 (2002).
34. X. Lopez, J.I. Mujika, G.M. Blackburn, M. Karplus
Alkaline Hydrolysis of Amide Bonds: Effect of Bond Twist and Nitrogen Pyramidalization.
Journal of Physical Chemistry A, **107**, 2304 - 2315, (2003).
35. J.I. Mujika, J.M. Mercero, X. Lopez
A Theoretical Evaluation of the pK_a for Twisted Amides Using Density Functional Theory and Dielectric Continuum Methods.
Journal of Physical Chemistry A, **107**, 6099 - 6107 (2003).
36. A.R. Dinner, X. Lopez, M. Karplus
A charge-scaling procedure to treat solvent in simulations.
Theor. Chem. Acc., **107**, 6099 - 6107 (2003).
37. X. Lopez, D.M. York
Parameterization of semiempirical methods to treat nucleophilic attacks to biological phosphates: AM1/d parameters for phosphorus Theor. Chem. Acc. (2003), 109, 149-159.
38. B.A. Gregersen, X. Lopez, D.M. York
Hybrid QM/MM study of thio effects in transphosphorylation reactions.
Journal of American Chemical Society, **125**, 7178 - 7179 (2003).
39. M.A.L. Marques, X. Lopez, D. Varsano, A. Castro and A. Rubio
Time-dependent Density-functional approach for biological chromophores: the case of the Green Fluorescent Protein.
Physical Review Letters, **90**, 258101-1 – 258101-4 (2003).
40. J.M. Mercero, J.I. Mujika, J.M. Matxain, X. Lopez, J.M. Ugalde
Incremental Binding Free Energies of Aluminum(III) vs Magnesium(II) complexes
Chemical Physics, **205**, 175 - 184 (2003).

41. E. V. Ludeña, J.M. Ugalde, X. Lopez, J. Fernández Rico and G. Ramírez
A reinterpretation of the nature of the Fermi hole
Journal of Chemical Physics, **120**, 540 - 547 (2004)
42. Kevin Range, Matthew McGrath, Xabier Lopez, Darrin M. York
The structure and stability of biological metaphosphate, phosphate and phosphorane compounds in the gas phase and in solution
Journal of American Chemical Society, **126**, 1654 - 1665 (2004).
43. A. Zubia, F.P. Cossío, I. Morao, M. Rieumont and X. Lopez
Quantitative Evaluation of the Catalytic Activity of Dendrimers with only One Active Center at the Core. Application to the Nitroaldol (Henry) Reaction.
Journal of American Chemical Society, **126**, 5243-5252 (2004).
44. J.M. Mercero, J.M. Matxain, E. Rezabal, X. Lopez and J.M. Ugalde
The First Solvation Shell of Aluminum (III) and Magnesium (II) Cations in a Protein Model Environment
International Journal of Quantum Chemistry, **98**, 409-424 (2004).
45. C. Silva López, O. Nieto Faza, B.A. Gregersen, X. Lopez, A.R. de Lera and D.M. York
Pseudorotation of Natural and Chemically Modified Biological Phosphoranes: Implications for RNA catalysis
Chem. Phys. Chem., **5**, 1045-1049 (2004).
46. B.A. Gregersen, X. Lopez, D.M. York
Hybrid QM/MM study of thio effects in transphosphorylation reactions: the role of solvation.
Journal of American Chemical Society, **126**, 7504–7513 (2004).
47. J.M. Mercero, J.M. Matxain, X. Lopez, D.M. York, A. Largo, L.A. Eriksson and J.M. Ugalde
Theoretical Methods that Help Understanding the Structure and Reactivity of Gas-Phase Ions
Review Paper in *Journal of Mass Spectrometry* (2005), **240**, 37-99. (Invited Review Article).
48. J.I. Mujika, J.M. Mercero and X. Lopez
Water-promoted hydrolysis of a highly twisted amide: Rate acceleration caused by the twist of the amide bond.
Journal of the American Chemical Society, (2005), **127**, 4445-4453.
49. Eduardo V. Ludeña, Xabier Lopez and Jesus M. Ugalde
Non-Born-Oppenheimer Treatment of the H₂ Hookean Molecule.
Journal of Chemical Physics (2005) accepted for publication.