

Curriculum vitae

Roberto LINGUERRI

Associate professor
Lab. LISIS/COSYS, Univ. Gustave Eiffel (UGE),
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Status and contact information

Nationality : Italian (48 yo)

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Formation

2016 HDR academic degree (French accreditation to supervise research) 30 November 2016.

Title of dissertation: **Determination of properties and spectroscopy of molecular systems of atmospheric and astrophysical interest.**

2003-2006 PhD thesis 7 Octobre 2006

Title : **Theoretical study of boron, silicon-carbon and sulfur clusters.**

Supervisor : **P. Rosmus** (LCT,UMLV,France).

Current position

Since April 2009

Associate professor at UGE

Selected scientific communications

1. Ghamri, M ; Harkati, D.; Belaidi, S.; Boudergua, S.; Ben Said, R.; Linguerri, R.; Chambaud, G.; Hochlaf, M.; Carbazole derivatives containing chalcone analogues targeting topoisomerase II inhibition: First principles characterization and QSAR modelling, Spectrochim. Acta A Mol. Biomol. Spectrosc. 242, 118724 (2020).
2. Boucenina, S.; Belkhir, L.; Meskaldji, S.; Linguerri, R.; Chambaud, G.; Boucekkine, A.; Hochlaf, M.; Electronic structure and magnetic properties of naphthalene- and stilbene-diimide-bridged diuranium(V) complexes: a theoretical study, J. Mol. Model. 26, 282 (2020).
3. Benabdelkrim, A.; Tourchi, A.E.; Hammoutene, D.; Ben Yaghlane, S.; Abdallah, H.H.; Linguerri, R.; Hochlaf, M.; Characterization of the simplest sulfenyl thiocyanate: isomers, spectroscopy and implications of astrophysical and biological relevance, Phys. Chem. Chem. Phys. 22, 17052-17061 (2020).

4. Al Harbi, S.D.A.; Al Mogren, M.M.; Elmarghany, A.; Ben Abdallah, D.; Mehnen, B.; Linguerri, R.; Hochlaf, M.; Gold with +4 oxidation state compounds: mass spectrometric and theoretical characterization of AuO²⁺, *Phys. Chem. Chem. Phys.* **21**, 16120 (2019).
5. Mohamed, D.; Ben Mohamed, F.E.; Amdouni, M.A.; Rhouma, M.B.; Linguerri, R.; Hochlaf, M.; Exploration of large amplitude motions in the Ca⁺Ar₂ complex, *Mol. Phys.* **117**, 1673 (2019).
6. Hendaoui, H.; Ben Abdallah, D.; Jaidane, N.E.; Al Mogren, M.M.; Almenia, S.; Elmarghany, A.; Linguerri, R.; Hochlaf, M.; Multi reference studies of gas phase vanadium nitride di- and trications, *Chem. Phys.* **517**, 113 (2019).
7. Mehnen, B.; Linguerri, R.; Ben Yaghlane, S.; Al Mogren, M.M.; Hochlaf, M.; Disentangling the complex spectrum of the ethynyl cation, *Farad. Disc.* **212**, 51 (2018).
8. Merabti, K.E.; Azizi, S.; Linguerri, R.; Chambaud, G.; Al-Mogren, M.M.; Hochlaf, M.; Electronic and Vibrational Spectroscopy of CsS, *J. Phys. Chem. A* **122**, 5354 (2018).
9. Gouid, Z.; Ben Said, R.; Sanhoury, M.A.; Boughdiri, S.; Prakash, M.; Linguerri, R.; Hochlaf, M.; Insights into the bonding between tributylphosphine chalcogenides and zinc(II), *Theor. Chem. Acc.* **137**, 68 (2018).
10. Liu, X.; Zhu, H.D.; Linguerri, R.; Han, Y.; Chambaud, G.; Meng, C.G., Interfacial-Bonding-Regulated CO Oxidation over Pt Atoms Immobilized on Gas-Exfoliated Hexagonal Boron Nitride, *CHEMISTRYSELECT* **2**, 9412 (2017).
11. Puzzarini, C.; Biczysko, M.; Peterson, K.A.; Francisco, J.S.; Linguerri, R., Accurate spectroscopic characterization of the HOC(O)O radical: A route toward its experimental identification, *J. Chem. Phys.* **147**, 024302 (2017).
12. Bonnet, L.; Linguerri, R.; Hochlaf, M.; Yazidi, O.; Halvick P.; Francisco, J.S., Full-Dimensional Theory of Pair-Correlated HNC O Photofragmentation, *J. Phys. Chem. Lett.* **8**, 2420 (2017).
13. Guo, H.M.; Li, M.; Liu, X.; Meng, C.G.; Linguerri, R.; Han, Y.; Chambaud, G., Fe atoms trapped on graphene as a potential efficient catalyst for room-temperature complete oxidation of formaldehyde: a first-principles investigation, *CATALYSIS SCIENCE & TECHNOLOGY* **7**, 2012 (2017) (sélectionné pour la couverture).
14. Deng, G.; Wu, Z.; Li, D.; Linguerri, R.; Francisco, J.; Zeng, X., The Simplest N-Sulfonylamine HNSO₂, *J. Am. Chem. Soc.* **138**, 11509 (2016).
15. Kutudila, P.; Linguerri, R.; Mogren Al-Mogren, M.; Pichon, C.; Condon, S.; Hochlaf, M., First principle investigations of organobismuth palladium-catalyzed C-C coupling reaction: mechanism, chemoselectivity and solvent effects, *Theor. Chem. Acc.* **135**, 176 (2016).
16. Sghaier, O.; Linguerri, R.; Mogren Al Mogren, M.; Francisco, J. S.; Hochlaf, M., Spectroscopic Constants of the X ¹Σ⁺ and 1 ³Π States of AlO⁺, *Astrophys. J.* **826**, 163 (2016).
17. Linguerri, R.; Puzzarini, C.; Francisco, J. S., Structure and Spectroscopic Properties of Low-lying States of the HOC(O)O radical, *J. Chem. Phys.* **144**, 084306 (2016).

18. Harrath, K.; Boughdiri, S.; Linguerri, R.; Hochlaf, M., Mechanistic study of bismuth-catalyzed direct benzylation of 2,4-Pentanediones: the case of BiCl₃ and generalization, *Theor. Chem. Acc.* 135, 2 (2016).
19. Trabattoni, A.; Klinker, M.; González-Vázquez, J.; Liu, C.; Sansone, G.; Linguerri, R.; Hochlaf, M.; Klei, J.; Vrakking, M. J. J.; Martín, F.; Nisoli, M.; Calegari, F., Mapping the dissociative ionization dynamics of molecular nitrogen with attosecond time resolution, *Phys. Rev. X* 5, 041053 (2015).
20. Bellili, A.; Linguerri, R.; Hochlaf, M.; Puzzarini, C., Accurate structural and spectroscopic characterization of prebiotic molecules: The neutral and cationic acetyl cyanide and their related species, *J. Chem. Phys.* 143, 184314 (2015).
21. Trabelsi, T.; Linguerri, R.; Ben Yaghlane, S.; Jaidane, N.-E.; Mogren Al-Mogren, M.; Francisco, J. S.; Hochlaf, M., On the role of HNS and HSN as light-sensitive NO-donors for delivery in biological media, *J. Chem. Phys.* 143, 134301 (2015).
22. Patanen, M.; Nicolas, C.; Linguerri, R.; Simoes, G.; Travnikova, O.; Liu, X. -J.; Hochlaf, M.; Bozek, J. D.; Miron, C., High-Resolution Photoelectron Spectroscopy with Angular Selectivity - A Tool To Probe Valence-Rydberg States and Couplings in HCl⁺, *J. Phys. Chem. A* 118, 4975 (2014).
23. Hochlaf, M.; Linguerri, R.; Francisco, J. S., On the role of the simplest S-nitrosothiol, HSNO, in atmospheric and biological processes, *J. Chem. Phys.* 139, 234304 (2013).
24. Delcey, M., G.; Lindh, R.; Linguerri, R.; Hochlaf, M.; Francisco, J. S., Theoretical prediction of the structure and spectroscopic properties of the X and A states of hydroxymethyl peroxy (HOCH₂OO) radical, *J. Chem. Phys.* 138, 021105 (2013).
25. Linguerri, R.; Hochlaf, M.; Bacchus-Montabonel, M.-C.; Desouter-Lecomte, M., Characterization of the MgO₂⁺ dication in the gas phase: electronic states, spectroscopy and atmospheric implications, *Phys. Chem. Chem. Phys.* 15, 824 (2013).
26. Hochlaf, M.; Linguerri, R.; Dalal, S. S.; Francisco, J. S., Theoretical study of the spectroscopically relevant parameters for the detection of HNP_q and HPN_q (q=0,+1,-1) in the gas phase, *J. Chem. Phys.* 136, 244311 (2012).
27. Linguerri, R.; Francisco, J. S., Coupled-cluster and multireference configuration interaction study of the low-lying excited states of the H₂O₂-H₂O complex, *J. Chem. Phys.* 137, 214312 (2012).
28. Mitrushchenkov, A. O.; Fano, G.; Linguerri, R.; Palmieri, P., On the importance of orbital localization in QC-DMRG calculations, *Int. J. Quantum Chem.* 112, 1606 (2012).
29. Mitrushchenkov, A. O.; Linguerri, R.; Chambaud, G., Piezoelectric Properties of AlN, ZnO, and Hg_xZn_{1-x}O Nanowires by First-Principles Calculations, *J. Phys. Chem. C* 113, 6883 (2009).
30. Mitrushchenkov, A. O.; Linguerri, R.; Rosmus, P.; Maier, J. P., Alternation of the spin-orbit coupling in the ²Π ground state of HC_nS (n=1-12) radicals, *Mol. Phys.* 107, 1549 (2009).
31. Rosmus, P.; Linguerri, R.; Komaha, N., First-Principle Computations of Rotational-Vibrational Transition Probabilities, *Mol. Phys.* 106, 2001 (2008).
32. Linguerri, R.; Komaha, N.; Fabian, J.; Rosmus, P., Electronic states of the Ultramarine Chromophore S₃⁻, *Z. Phys. Chem.* 222, 163 (2008).

33. Cheng, M.; Brown, J. M.; Rosmus, P.; Linguerri, R.; Komihara, N.; Myers, E. G., Dipole Moments and Orientation Polarizabilities of Diatomic Molecular Ions for Precision Atomic Mass Measurement, *Phys. Rev. A* 75, 012502 (2007).
34. Linguerri, R.; Rosmus, P.; Carter, S., Anharmonic vibrational levels of the two cyclic isomers of SiC₃, *J. Chem. Phys.* 125, 034305 (2006).
35. Linguerri, R.; Navizet, I.; Rosmus, P.; Carter, S.; Maier, J. P., Vibrations in the B₄ rhombic structure, *J. Chem. Phys.* 122, 034301 (2005).
36. Mitrushenkov, A. O.; Fano, G.; Ortolani, F.; Linguerri, R.; Palmieri, P., Quantum chemistry using the density matrix renormalization group, *J. Chem. Phys.* 115, 6815 (2001).

Summer school

CAPZEO-2014: The Fourth International Summer School On Quantum Electronic Calculations, Introduction to ab initio Chemistry with MOLPRO, Université Mohammed V-Agdal, Rabat, 9 juin 2014.

Direction of publications

- Hochlaf, M.; **Lingerri, R.**; Lauvergnat, D., PCCP themed issue (volume 15, 22 Mai 2013) *Spectroscopy and dynamics of medium-sized molecules and clusters: theory, experiment and applications*, RSC Publishing (2013) (co-editor).

Organisation of scientific meetings

- Member of the organizing committee of the presentation conference of Prof. J. S. Francisco at the Université Paris-Est (11th July 2016), for his scientific project with Université Paris-Est Marne-la-Vallée.
- Member of the organizing committee of **1st MOLIM General Meeting** (action COST CM1405: Molecules in motion (MOLIM)), Université Paris Est - Marne la Vallée, 27-29 August, 2015.
- Member of the scientific committee of the workshop *Capture and storage of atmospheric pollutants: microscopic studies and applications*, European project CapZeo, PF7 Marie Curie IRSES, Madrid (Spain), 24th april 2015 (<http://tct1.iem.csic.es/CAPZEO.htm>).
- Member of the organizing committee of **AMOC 2015, Anharmonicity in medium-sized molecules and clusters**, CSIC, Madrid (Spain), 26-30 April, 2015.
- Member of the scientific and organizing committees of **CAPZEO-2014: The Fourth International Summer School On Quantum Electronic Calculations**, Université Mohammed V-Agdal, Rabat, 9-12 June 2014.
- Member of the scientific board and of the organizing committee of the workshop : **CAPZEO 2013, International symposium on CO₂ capture: Microscopic studies and applications**, Champs-sur-Marne, 18-20 September 2013, 21 invited speakers, 67 participants.

- Member of the organizing committee of : **AMOC 2012**, *Anharmonicity in medium-sized molecules and clusters*, Champs-sur-Marne, 18-21 Avril 2012, 125 participants from 18 countries.
- Member of the organizing committee of : **JIREC 2013**, *29^e Journées pour l'Innovation et la Recherche dans l'Enseignement de la Chimie : Enseigner une Chimie Économe et Créatrice*, Université de Marne-la-Vallée, 21-24 mai 2013, 120 participants.