UNIVERSITÀ DEGLI STUDI DI MILANO

TO MAGNIFICO RETTORE OF UNIVERSITA' DEGLI STUDI DI MILANO

I the undersigned asks to participate in the public selection, for qualifications and examinations, for the awarding of a type A post-doc fellowship

[Nabil Omri]

CURRICULUM VITAE

PERSONAL INFORMATION

Surname	Omri
Name	Nabil
Date of birth	[23, October, 1982]

PRESENT OCCUPATION

Appointment	Structure
Postdoctoral Researcher	School of Chemistry and Chemical Engineering, Shandong University, China

EDUCATION AND TRAINING

Degree	Course of studies	University	year of achievement of the degree
Degree	High Level Diploma in Chemical Engineering	Tunis ElManar	2005
Specialization	National Engineering Degree in Chemistry	Tunis ElManar	2009
PhD	PhD of Philosophy in Chemistry	Paris-Saclay / Tunis ElManar	2017
Master	Master's Degree in Chemistry	Tunis ElManar	2011
Degree of medical specialization			
Degree of European specialization			
Other			

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REGISTRATION IN PROFESSIONAL ASSOCIATIONS

Date of registration	Association	City
2017	Membre of the Association of Heterocyclic Chemistry and Applications "STCHA"	Tunis

FOREIGN LANGUAGES

Languages	level of knowledge
Arabic	Native
French	Native
English	Native

AWARDS, ACKNOWLEDGEMENTS, SCHOLARSHIPS

Year	Description of award
2012	PhD fellowship founded by IUT of Orsay (Paris 11 University), France
2018	Postdoctoral Researcher, High Level Foreign Talents Program, Chinese Government

TRAINING OR RESEARCH ACTIVITY

Considering the significant potential of cyclopropanation or 1,3-dipolar cyclo-addition of azomethine ylides to C60, the aim of the my PhD thesis was studying the feasibility of irradiating C60 and amino acid reaction medium to develop a new nanovector generation. Indedd, the project proposed another pathway to synthesize multifunctional nanocarriers, using 1,3-dipolar [3+2] photo-cycloaddition reactions. In this strategy, two reaction mechanisms were theoretically proposed and experimentally verified for the addition of tryptophan methyl ester (TrpME) on C60. It has been found that the cycloaddition through photoexcitation is preceded on the triplet state surface instead of the singlet ground state energy surface. Regarding their two pathways in singlet and triplet PES, using B3LYP/6-31+G(d,p)/LANL2DZ, it is clear that the FPL mono-adduct is thermodynamically the most favorable under excitation. In fact, when, the azomethine ylide is combined with C60, two CC bonds are created with an activation barrier of about 1.92 kcal/mol in the triplet state.

After my selection by the High Level Foreign Talents Program of Chinese Government, as a postdoctoral researcher, I joined the research group of Prof. Dr. Yuxiang BU, at the department of theoretical chemistry at the School of Chemistry and Chemical Engineering of Shandong University. During this period our research is focused on three important points:

- Electronic Structures and Nonlinear Optical Properties of the Single Vacancy-Defected [60]Fullerene (C59[9-4] and C59[8-5] Isomers of the C59 cluster): We conduct in this work an in-depth investigation on the stability, electronic, photophysical and nonlinear optical properties of the single vacancy-defected C60 isomers by quantum chemistry and wavefunction analyses. This first exploration, in static and dynamic regimes, can help us understanding the effect of symmetry, even and odd-electron systems as well as molecular topology on the electronic and optical nonlinearity of both the C59[9-4] and C59[8-5] isomers. It is found that the frequency-dependent polarizability anisotropy αanisotropy (λ = 1064.80 nm) of C59[8-5] is 4 times larger than the static regime, revealing a notable polarization anisotropy, due to the delocalized π electrons around the vacancy defect. By decreasing the incident wavelengths from λ = 1908 nm to λ =589.08 nm, the dispersion of optical nonlinearity of C59 [8-5] has achieved the maximum

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at βxxx (λ = 1064.8 nm) = 38.150 au and (γxxxx (λ = 589.08 nm) = −9.896 × 107 au), indicating that the resonance effect of the hyperpolarizability amplified with the decrease of incident wavelengths.

- TD-DFT investigation on Single and Double Vacancy Defected Endohedral Metallofullerene-Superhalogen Anions: Molecular Topology and Nonlinear Optical Property of Na@C59[9-4]([8-5])-AlX4 and Na@C58-AlX4 (X = Cl, Br) Compounds: Continuing our interest in studying the unusual topology of both isomers, we will report in this future publication a theoretical prediction on the influence of superatom character of Na@C59-AlX4 and Na@C58-AlX4 (X = Cl, Br) on the topology, electronic properties and molecular optical nonlinearity responses of their compounds.

- The functionalization of [60]Fullerene, though 1,3 dipolar [3+2] Photo-cycloaddition for Anticancer Drug Delivery Nanovector Synthesis.

- The Feasibility of Functionalizing [60]Fullerene and [60]Boron-Nitride Systems, to Develop Suitable Nanocarriers for Anticancer Drugs.

PROJECT ACTIVITY

Year	Project
2012	Functionalization of [60]Fullerene through photochemical reaction: Theoretical investigations on the fulleropyrrolidine nanovectors synthesis.
2017	Development of metal hydroxide nanoparticles and their application as flame retardants for ethylene-vinyl acetate copolymer (EVA): Theoretical and Experimental Approaches
2018	Theoretical Investigations on Novel Carbon Based-Nanomaterials Derivatives for Biomedical Applications: Electronic Properties and Optical Nonlinearity Responses.

PATENTS

Patent

CONGRESSES AND SEMINARS

Date	Title	Place
April, 16-17th 2018	Participation at the training: Modeling Applied to Catalysis, Prof. Dr. Carine Michel, CNRS, France.	Paris
May 16th 2017	First Maghreb Colloquium on the heterocyclic chemistry: Mechanism and number of adducts of photo-addition reaction of Tryptophan methyl-ester on [60]Fullerene.	Tunis
May, 17th 2017	First Maghreb Colloquium on the heterocyclic chemistry: Theoretical study of the addition of Tryptophan methyl-ester on [60]Fullerene: Structures and Mechanisms.	Tunis
June, 1st 2016	First International Days of heterocyclic chemistry and its applications: HF and DFT investigations on the synthesis mechanism and conformational stability of N'-Formylkynurinine.	Tunis
March, 16-18th 2015	17th Arab Chemistry Conference: Fonctionalization of [60]Fullerene by [2+3]photocycloaddition reaction: Synthesis and Characterization of Fulleropyrrolidine derivatives.	Tunis

December, 21-23th 2014	National Days of Chemistry- JNC 2014- 18th Edition:	Tunis
June, 5th 2014	"From one extreme to the other" held at the School of Industrial Physics and Chemistry of Paris (ESPCI ParisTech), Paris, France, by the Club AFSEP, Ile de France, local branch of the French Association of Separation Sciences (AFSEP).	Paris
April, 2-3th 2014	Participation at the 4th School of Molecular Physics:	Tunis

PUBLICATIONS

Books
[title, place, publishing house, year ...]
[title, place, publishing house, year ...]
[title, place, publishing house, year ...]

Articles in reviews
Nabil OMRI, Yuxiang BU. TD-DFT Studies on sp and sp^2 Hybridized Single Vacancy-Defected [60]Fullerene: Electronic Excitation and Nonlinear Optical Properties of both C59[9-4] and C59[8-5] Isomers. *J. Phys. Chem. A* 2021, 125, 106-114. https://pubs.acs.org/doi/10.1021/acs.jpca.0c08533
Nabil OMRI, Fathi MOUSSA, Yuxiang BU. Functionalization of [60]Fullerene through Photochemical reactions for Fulleropyrrolidine nanovectors synthesis: Experimental and theoretical approaches. *Colloids. Surf. B. Biointerfaces*. 2020, 111457. https://www.sciencedirect.com/science/article/pii/S0927776520308134
Nabil OMRI, Yuxiang BU. Azomethine ylide addition impact on functionalized [60]Fullerene and [60]Boron-Nitride: Anticancer Doxorubicin and Boronic Chalcone drugs binding characteristics with mono- and bis-nanocarriers, *Colloids. Surf. B. Biointerfaces*. 2020, *196*, 111277. https://www.sciencedirect.com/science/article/abs/pii/S0927776520306330
Nabil OMRI, Mohamed amine OUALHA, Loic BRISON, Henri VAHABI, Fouad LAOUTID. Novel nanocomposites based on EVA/PHBV/[60]Fullerene with improved thermal properties, *Polym. Test.* 2020, *81*, 106277. https://www.sciencedirect.com/science/article/pii/S014294181831643X
Mohamed amine OUALHA, Nabil OMRI, Rafeh OUALHA, Mohamed Anouar NOUIOUI, Manef ABDERRABBA, Noureddine AMDOUNI, Fouad LAOUTID. Development of metal hydroxide nanoparticles from eggshell waste and seawater and their application as flame retardants for ethylene-vinyl acetate copolymer (EVA). *Inter. J. Biol. Macromol*, 2019, *128*, 994-1001. https://www.sciencedirect.com/science/article/pii/S0141813018331945
Nabil OMRI, Mohamed amine OUALHA, Henri VAHABI, Noureddine AMDOUNI, Manef ABDERRABBA, Fouad LAOUTID. Promising effect of combining [60]Fullerene nanoparticles and calcium hydroxide on thermal stability and flammability of Poly(ethylene-co-vinyl acetate). *Thermochim. Acta*. 2018, *668*, 73-79. https://www.sciencedirect.com/science/article/pii/S004060311830306X?via%3Dihub
Nabil OMRI, Noura KHEMIRI, Fathi MOUSSA, Manef ABDERRABBA, Sabri MESSAOUDI. Addition of Tryptophan-Methyl Ester on [60]Fullerene: Theoretical investigation on the mechanisms of Azomethine Ylides and Fulleropyrrolidine formation. *J. Mol. Model*, 2018, *24*, 270. https://link.springer.com/article/10.1007%2Fs00894-018-3760-2
Nabil OMRI, Mohammed YAHYAOUI, Ridha BANANI, Sabri MESSAOUDI, Fathi MOUSSA, Manef ABDERRABBA. Ab-initio HF and Density Functional Theory Investigations on the synthesis mechanism, conformational stability, molecular structure and UV spectrum of N'- Formylkynurenine. *J. Theor. Comput. Chem.* 2016, *15*, 1650006. https://www.worldscientific.com/doi/abs/10.1142/S0219633616500061
Dorra MAHDAOUI, Chika HIRATA, Nabil OMRI, Takatsugu WAKAHARA, Manef ABDERRABBA, Kunichi MIYAZAWA. Optimization of the liquid-liquid interfacial precipitation method for the synthesis of C60 nanotubes. *Bull. Mater. Sci.* 2018, *41*, 165. https://link.springer.com/article/10.1007%2Fs12034-018-

1665-4
Ridha BANNANI, Abdelkarim AYDI, Nabil OMRI, Mounir BEZARGUA, Manef ABDERRABBA. Optimization of the pretreatment step conditions for biodiesel production from waste frying oil using Box-Behnken design. *J. Mater. Environ. Sci.* 2016, 7, 4348-4360. https://www.jmaterenvironsci.com/Document/vol7/vol7_N12/462-JMES-2602-Ridha.pdf
[title of the article, review, place, publishing house, year ...]

Congress proceedings
[title, structure, place, year]
[title, structure, place, year]
[title, structure, place, year]

OTHER INFORMATION

Declarations given in the present curriculum must be considered released according to art. 46 and 47 of DPR n. 445/2000.

The present curriculum does not contain confidential and legal information according to art. 4, paragraph 1, points d) and e) of D.Lgs. 30.06.2003 n. 196.

Place and date: _____Shandong, China_____, _August, 23rd 2021_____

SIGNATURE

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