



### 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

[Name and surname] Kazem Zhour CURRICULUM VITAE

#### PERSONAL INFORMATION

Surname	Zhour
Name	Kazem
Date of birth	[30, 10, 1988]

#### PRESENT OCCUPATION

Appointment	Structure
Visiting researcher	Laboratoire de Chimie et Physique Approche Multi-échelles des Milieux Complexes (LCP-A2MC) Université de Lorraine.

#### EDUCATION AND TRAINING

Degree	Course of studies	University	year of achievement of the degree
PhD	Condensed matter physics	Lebanese University and K. N. Toosi university of technology	Mar. 2021
Master's degree	Nano-science and functional materials	Lebanese University	July 2011
Bachelor's Degree	Physics	Lebanese University	October 2009

#### FOREIGN LANGUAGES

Languages	level of knowledge	
Arabic	Native	
English	Fluent	
French	Fluent	



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Persian	Fluent	
Spanish	Basics	

#### AWARDS, ACKNOWLEDGEMENTS, SCHOLARSHIPS

Year	Description of award
2019	Erasmus mobility to the facultad de física- Universidad de Santiago de Compostela - Santiago de Compostela - Spain
2020	Erasmus mobility to the Laboratoire de Chimie et Physique Approche Multi-échelles des Milieux Complexes (LCP-A2MC) Université de Lorraine

#### TRAINING OR RESEARCH ACTIVITY

• My PhD thesis (defended in March 4, 2021) was done under double supervision of **Prof. Fouad El Haj Hassan** (Lebanon University, Beirut) and Prof. Majid Vaezzadeh (K. N. Toosi University of technology, Teheran), so that I'll receive a joint degree of these both universities. The manuscript of my thesis is available at my profile on researchgate (researchgate.net/profile/Kazem-Zhour).

• I studied Ramanand IR spectroscopy of different sizes of graphene quantum dots using Gaussian09. The work was published in "Journal of Interfaces, Thin Films and Lowdimensional systems". Right now, I am preparing another manuscript that considered the effect of the adsorption of potassium atoms on the graphene quantum dots.

• I studied the effect of doping the graphene sheet with the boron and nitrogen atoms on the adsorption of potassium atom and the effect on the electronic and magnetic properties of the obtained system. The calculation was all done using quantum espresso code, and I used Xcrysden to visualize the systems and sigma plot for graphical representations. This work was published in the "Materials Today Communications".

• During my Erasmus mobility to the university of Santiago de Compostela in Spain under the supervision of **Prof Luis Miguel Varela**, I worked on the effect of the existence of the ionic liquid near the graphene and Pmmn8 borophene (another 2D material with Dirac cone) on their electronic (DOS, band structure, charge transfer, ...) and optical properties (dielectric functions, electron energy loss spectroscopy, index of refraction, adsorption coefficient, ...). Later I considered the effect of adding potassium atom to the mixture. This work resulted in two publications in the "Journal of Molecular Liquids". All the calculations were done using the quantum espresso package, Xcryden, visual molecular dynamics (vmd), xmgrace and python were used to visualize and treat the obtained outputs. Right now, me and the group of Prof. Luis are considering a wide range of metal additives to study their effect and compared with that of potassium, and I am helping my wife in here thesis with professor Luis to consider the case of lonic liquid adsorbed on multilayer graphene.

• During my Erasmus mobility to the University of Lorraine in France under the supervision of **Prof Andrei Postnikov**, I worked with him on the graphene-like BC3 where we studied the interaction between two potassium atoms adsorbed on the sheet. This work was done using Siesta code, and some calculations were done using quantum espresso for comparative reasons. It is right now under submission in the journal "physica status solidi. Right now, we are planning to collaborate with other colleagues in the university of Lorraine to extend this study.

• I am also collaborating with my colleagues, Dr. Wael Chmaisani (BAU university, Lebanon), in the thesis of a master student which study the electric properties of doped NiO crystals and nanostructure to compare the result from our DFT calculation to experimental results obtained by the student.

• Recently, I start studying the adsorption of some gases on 2D materials sheet in collaborating with **Dr**. **Micheal Badawi** from the LCP laboratory in the university of Lorraine. In this study I am using VASP to accomplish all the calculation needed.



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• I am also collaborating with the experimental members of the group to calculate the Raman spectroscopy of zinc blende crystals with dopant using quantum espresso as it has the capability to split the LO and TO modes of vibration. We found that it may be helpful to generate our own prepotential files to get results in more agreement with the experimental values, therefore I am currently working on generating these pseudopotentials using atomic; program was implanted in the quantum espresso package.

For my participations in international and national workshops, schools, and my seminars please check "Domanda" file.

Date	Title	Place		
Seminars:				
8 Jul. 2021	Theoretical mapping of interaction between alkali metal atoms adsorbed on graphene-like BC3 monolayer	Laboratoire de Chimie et Physique Approche Multi-échelles des Milieux Complexes (LCP- A2MC) Université de Lorraine - Metz - France		
16 Oct. 2020	Ionic Liquid on 2D material: electronic and plasmonic properties of hybrid interface.	Laboratoire de Chimie et Physique Approche Multi-échelles des Milieux Complexes (LCP- A2MC) Université de Lorraine - Metz - France		
15 Oct. 2019	Quantum espresso workshop: DFT and TD- DFT calculations	Universidad de Santiago de Compostela - Santiago de Compostela -Spain:		
13 Sep. 2019	Plasmonic properties of graphene with DFT and TD-DFT calculation	Universidad de Santiago de Compostela - Santiago de Compostela -Spain:		
Schools and	Schools and Workshops:			
28 Jun 2 Jul. 2021	SIESTA school "First-principles simulations of materials with SIESTA".	CECAM (online)		
14-18 Jun. 2021	2021 Virtual School on Electron-Phonon Physics and the EPW code.	Texas (online)		
7 Jun. 2021	QuantumATK S-2021.06 Release: Highlights of New Features and Enhancements ().	online		
24-28 May 2021	Workshop on Physics and Chemistry of Solid/Liquid Interfaces for Energy Conversion and Storage,	ICTP, Trieste, Italy (online)		
3 May 2019	2nd National Workshop on Innovative Materials and Applications (NWIMA -2) - Lebanese. Poster: "Adsorption of Carbon Monoxide on Doped Graphene".	University - Fanar - Lebanon		

### CONGRESSES AND SEMINARS

PUBLICATIONS

#### Articles in reviews

[Theoretical mapping of interaction between potassium atoms adsorbed on boron carbide monolayer, physica status solidi, 2021]

[Tuning the hybrid borophene-/graphene-ionic liquid interface: Effect of metal cations on the electronic and photonic properties, Journal of Molecular Liquids, 2020]

[Electronic and optical properties of borophene and graphene with an adsorbed ionic liquid: A density



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functional theory study, Journal of Molecular Liquids, 2020]

[DFT study of Benzene, Coronene and Circumcoronene as zigzag graphene quantum dots, Journal of Interfaces, Thin Films and Low dimensional systems, 2019]

[Ab initio study of the adsorption of Potassium on B, N, and BN-doped graphene heterostructure, Materials Today Communications, 2019]

#### OTHER INFORMATION

From 2012 to 2016

Teacher of physics in Lebanese high schools for all grades and branches.

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: 23 Metz-France, 20/7/2020

SIGNATURE

Kazem Zhour

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