TO MAGNIFICO RETTORE OF UNIVERSITA' DEGLI STUDI DI MILANO **ID CODE __5853_____**

I the undersigned asks to participate in the public selection, for qualifications and examinations, for the awarding of a type B fellowship at **Dipartimento di _____Fisica Aldo Pontremoli_____**

Scientist- in – charge: **_____Dott.ssa Achilli_____**

[Name and surname]

CURRICULUM VITAE

PERSONAL INFORMATION

Surname	Shahrokhi
Name	Masoud

PRESENT OCCUPATION

Appointment	Structure
Research Associate 2022-present	ICGM, Univ. Montpellier, France,

EDUCATION AND TRAINING

Degree	Course of studies	University	year of achievement of the degree
Degree			
Specialization			
PhD	Condensed matter theory	Razi University	2014
Master	Condensed matter theory	Kharazmi University	2011
Degree of medical specialization			
Degree of European specialization			
Other			

REGISTRATION IN PROFESSIONAL ASSOCIATIONS

Date of	Association	City

registration		

FOREIGN LANGUAGES

Languages	level of knowledge
English	Advanced
Persion	Native
French	Basic

AWARDS, ACKNOWLEDGEMENTS, SCHOLARSHIPS

Year	Description of award
2022-present	Research Associate : ICGM, Univ. Montpellier, France,
2021-2022	Research Associate: IFP Energies nouvelles, Lyon, France
2019-2021	Research Associate: École normale supérieure de Lyon, France
2018-2019	Research Associate: Razi University, Kermanshah, Iran
2016-2018	Research Associate: Institut Català d'Investigació Química (ICIQ), Spain
2015-2016	Research Associate: University of Paris-Est, France

TRAINING OR RESEARCH ACTIVITY

description of activity

I am writing to express my keen interest in a research position in computational material properties within your esteemed group. I am confident that my expertise in density functional theory (DFT) and my strong research background make me a suitable candidate for this position.

I hold a Ph.D. degree in Condensed Matter Physics, which I received in 2014. During my doctoral studies, I focused on investigating the electronic and optical properties of semiconductors and insulators, specifically ZnO and BeO nanomaterials, using various software platforms such as Wien2K and Exciting. I achieved the 1st rank among all graduated Ph.D. students, attaining a remarkable GPA of 19.68 out of 20. Additionally, I gained valuable experience by collaborating with Prof. R. Dovesi's group at Torino University, where I investigated the thermodynamic properties of materials using the CRYSTAL code.

Following my Ph.D., I worked as a postdoctoral fellow at the University Paris-Est Marne-la-Vallée for a year (2015-2016), where I focused on multiscale chemo-mechanical modeling of graphene-coated materials. During this period, I extensively utilized DFT to model the structure and stability of carbon clusters and organic molecules on Cu (111) surfaces. I also studied the electronic and optical properties of semiconductors using GW and BSE methods implemented in the VASP code. The outcomes of these projects were successfully published in renowned journals such as the Journal of Alloys and Compounds and Applied Surface Science.

Subsequently, I joined the computational chemistry group at Institut Català d'Investigació Química (ICIQ) as a postdoctoral fellow from 2016 to 2018. In this role, I focused on simulating new families of hydrogenation catalysts based on ligand-modified nanoparticles and alloy and intermetallic systems. Our research demonstrated the exceptional activity, selectivity, and stability of ligand-modified Pd nanoparticles in direct H2O2 synthesis. Additionally, our studies revealed the intriguing geometric and electronic characteristics, as well as high stability, of supported palladium sulfides as catalysts for selective hydrogenation of alkynes. These findings were published in prestigious journals such as Nature Communications and Angewandte Chemie International Edition.

From 2018 to 2019, I worked at Razi University in Iran, researching the geometry and optoelectronic properties of novel 2D materials. During this time, I collaborated closely with Prof. Rabczuk's group at Bauhaus Universität-Weimar, resulting in several publications in renowned journals including Carbon, Nanoscale, Journal of Material Chemistry A, Applied Materials Today, Journal of Materials Chemistry C, Nanotechnology, and Journal of Alloys and Compounds. I focused on investigating the structural, mechanical, electronic, and optical properties of novel 2D semiconductors and metallic materials.

From 2019 to 2021, I conducted research at ENS-Lyon, where I explored the potential of 2D semiconductor materials for photocatalytic applications. I measured various physical properties, such as electronic bandgap, dielectric function, charge carrier mobility, absorption coefficient, and exciton binding energy, to evaluate their suitability for photocatalysis, particularly water splitting. My project involved predicting the optoelectronic properties of bulk MoO 3-xSx and MoS 2-xOx layered materials using DFT-HSE formalism. Additionally, I extended this study to the case of finite-layer systems, implementing a specific method to investigate the evolution of dielectric constant in such systems.

From February 2021 to August 2022, I held a postdoctoral researcher position at IFP Energies Nouvelles, collaborating closely with Ecole Normale Supérieure de Lyon. During this period, my focus was on conducting research activities within the framework of a project named "Reactivity of supported platinum-based nanoclusters investigated by DFT," which received funding from the ROAD4CAT chair. This project involved studying the behavior of highly ductile monometallic platinum and platinum-tin clusters supported on gamma-alumina. To address the complexities of these systems, I employed a combination of ab initio molecular dynamics (AIMD) simulations and transition state (TS) search methods. The objectives of the project encompassed refining existing models and examining the mechanistic aspects of methylcyclohexane dehydrogenation.

Starting from December 2022, I have been employed as a postdoctoral researcher at ICGM, CNRS Montpellier. My current research focuses on the investigation of "supported catalytically active liquid metal solutions" (SCALMS). To explore this area, I will be utilizing DFT calculations to analyze the energetic stabilities, geometric configurations, and electronic structures of Pt when highly diluted with metals M (M = Ga, Sn, Cu). This analysis will involve extended flat surface models as well as small nanoparticles, considering the presence of adsorbates such as propane, N2, and H2. In order to define

the stability phase diagram (T, P) of highly diluted Pt, I will model environmental Pt surface segregation, reverse segregation towards the bulk, and sintering phenomena as a function of temperature and gas pressure. Additionally, I plan to perform ab initio molecular dynamics simulations under various temperature and pressure conditions to investigate the atomic-scale structures of promoters in both solid and liquid states, with ultra-low Pt concentrations. By computing binding energies and conducting frequency calculations, I will conduct an in-depth analysis of the electronic structure and reactivity of these systems towards probe molecules. Moreover, I aim to employ the selected active materials to identify the reaction pathway and elementary steps involved in the partial dehydrogenation (PDH) reaction taking place at the catalyst's surface. Through these investigations, I intend to gain a comprehensive understanding of the SCALMS system and provide valuable insights into its catalytic behavior and mechanisms.

My research interests predominantly revolve around nanotechnology, semiconductors, optoelectronic properties, magnetic properties, heterogeneous catalysis, and heterostructures. I possess significant expertise in performing calculations based on Density Functional Theory, GW and BSE methods, NEB calculations, and molecular dynamics simulations. I am proficient in various codes, including full-potential Linearized Augmented Plane Wave (LAPW) and pseudo-potential PW and Projected Augmented Wave (PAW) codes such as WIEN2K, Exciting, Quantum ESPRESSO, VASP, as well as Gaussian-type orbital basis sets codes like CRYSTAL and CP2K.

PROJECT ACTIVITY

Year	Project
2022-present	Research Associate : ICGM, Univ. Montpellier, France, Performing research on the supported catalytically active liquid metal solutions (SCALMS) by AIMD and DFT in the group of Dr. Hazar Guesmi.
2021-2022	Research Associate: IFP Energies nouvelles, Lyon, France Performing research on the Reactivity of supported platinum-based nanoclusters investigated by DFT in the group of Dr. Pascal Raybaud.
2019-2021	Research Associate: École normale supérieure de Lyon, France Performing research on the predicting the optoelectronic properties of 2D and 3D layered materials such as MoS2 and MoO3 in the group of Dr. Pascal Raybaud and Dr. Tangui Le Bahers.
2018-2019	Research Associate: Razi University, Kermanshah, Iran Performing research on the novel optoelectronic 2D materials in the group of Prof. Rostam Moradian.
2016-2018	Research Associate: Institut Català d'Investigació Química (ICIQ), Spain Performing research on the catalytic materials (metallic surfaces) within the framework of a Marie Curie–COFUND in the group of Dr. Nuria Lopez.

2015-2016	Research Associate: University of Paris-Est, France Performing research on the multiscale chemo-mechanical modeling of graphene-coated materials. Performing research on the electronic and optical properties of semiconductors by using GW and BSE methods by using VASP in the group of Prof. Céline LEONARD.
2014	Visiting researcher: Dipartimento di Chimica, Universita di Torino and NIS, Italy Performing research on the thermodynamic properties of materials using CRYSTAL code in the group of Prof. Roberto Dovesi.
2011-2014	Ph.D. in Condensed Matter Physics: Razi University, Kermanshah, Iran Ph.D. thesis: Zinc oxide and Beryllium oxide Nanostructurs

PATENTS

Patent

CONGRESSES AND SEMINARS

Date	Title	Place

PUBLICATIONS

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

Articles in reviews
I have more than 65 published papers. For the complete list please refer to my Google Scholar: https://scholar.google.com/citations?user=5yNqdK4AAAAJ&hl=en

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.

Please note that CV WILL BE PUBLISHED on the University website and It is recommended that personal and sensitive data should not be included. This template is realized to satisfy the need of publication without personal and sensitive data.

Please DO NOT SIGN this form.

Place and date: Montpellier, 14/08/2023