



TO MAGNIFICO RETTORE OF UNIVERSITA' DEGLI STUDI DI MILANO PNRR - Prof. Guerra ID CODE 6907

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

Scientist- in - charge: Dr. Prof. Roberto Guerra

[Somayeh Ahmadkhani]

## CURRICULUM VITAE

### PERSONAL INFORMATION

Surname	Ahmadkhani
Name	Somayeh

### PRESENT OCCUPATION

Appointment	Structure
Postdoc researcher	Poland - Torun, UMK

### EDUCATION AND TRAINING

Degree	Course of studies	University	year of achievement of the degree
PhD	36	University of Zanjan	February 2020
Master	42	IASBS	April 2015
Bachelor	120	University of Zanjan	July 2012

### REGISTRATION IN PROFESSIONAL ASSOCIATIONS

Date of registration	Association	City



## FOREIGN LANGUAGES

Languages	level of knowledge
English	B2
Germany	A1

## AWARDS, ACKNOWLEDGEMENTS, SCHOLARSHIPS

Year	Description of award
2022	The best researcher at the Shahid Rajaei teacher training university

## TRAINING OR RESEARCH ACTIVITY

My research aims to explore novel quantum effects in materials with flat bands, conduct DFT calculations of oxidized monolayer graphene, investigate water flow properties through carbon nanotubes with molecular dynamic simulations (LAMMPS) , and utilize the USPEX package for structure prediction and using quantum chemistry methods for studying properties of molecular structures.

I am currently collaborating with a chemical physics group as a two-year postdoc researcher (2 month left). My work focuses on linear response calculations and excited dipole moment analysis for molecular structures. I have completed my research and am revising submission. Additionally, I am supervising two Ph.D. students. I am also working on implementing expectation dipole moment calculations in the PyBEST package.

## PROJECT ACTIVITY

Year	Project
2022-2025	Postdoc researcher in Poland, Torun ;“ Development of pCCD-based methods to reliably model electronic structures and properties of building blocks of organic solar cells.”
2021-2022	Postdoc researcher in Iran, Tehran; “ DFT calculations on oxidized mono layer graphene.”
2022	Visiting researcher Poland, Torun; “Derivation and implementation of the linear response function on the pCCD model.”



## PATENTS

Patent

## CONGRESSES AND SEMINARS

Date	Title	Place
1-5.September.2024	CTTC IX (ninth edition of the Current Trends in Theoretical Chemistry conference)	Krakow, Poland —> Talk
9-12 July 2024	IMAMPC (13th International Meeting on Atomic and Molecular Physics and Chemistry)	Warsawa —> Poster
June 26-July 1 2023	17th International Congress of Quantum Chemistry (ICQC)	Bratislava —> Poster
1-2 June 2023	Young Science Beyond Borders (YSBB), Poland (Online)	Poland —> Talk
25 March 2021	<i>Mini- Workshop</i> towards strong correlations in van der waals heterostructures and 2d materials, Nanoscale Coherent Hybrid Devices for Superconducting Quantum Technologies	Online
22 April 2021	<i>31st International Conference on Diamond and Carbon Materials, Boosting Superconductivity in 2D materials by beneficial defects, CEST (Online),</i>	Online —> Talk

## PUBLICATIONS

Papers
PyBEST: Improved functionality and enhanced performance”, Computer Physics Communications <b>297</b> , 109049 (2024)
Multi-band flattening and linear Dirac band structure in graphene with impurities” Phy.Rev.B <b>107</b> , 075401(2023)
Electronic Properties of Oxidized Graphene: Effects of Strain and an Electric Field on Flat Bands and the Energy Gap, J. Phys. Chem. Lett. <b>13</b> , 1, 66–74 (2022)
Superconducting proximity effect in flat band systems, J. Phys. Condense. Matter <b>32</b> 315504 (2021)

Articles in reviews
Linear response pCCD-based methods: LR-pCCD and LR-pCCD+S approaches for the efficient and reliable modelling of excited state properties, review, Journal of Chemical Theory and Computation, 2024



Congress proceedings
Simple and efficient computational strategies for calculating orbital energies from pCCD and orbital-optimized pCCD methods., PCCP, 2024
Extended Koopmans pCCD orbital energies, PCCP, 2024
Expectation Dipole Moments with pCCD, JCTC, 2024
Huckel and PPP model Hamiltonian effects on pCCD excitation energies....

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: Poland-Toruń, 03.10.2024