AL MAGNIFICO RETTORE
DELL'UNIVERSITA' DEGLI STUDI DI MILANO

[Elaheh Mohebbi]

CURRICULUM VITAE

INFORMAZIONI PERSONALI

Cognome	Mohebbi
Nome	Elaheh
Data Di Nascita	[29, 08, 1981]

OCCUPAZIONE ATTUALE

Incarico	Struttura
Post-Doc Researcher 9/2019- Present Main responsibilities: a. High-throughput ab-initio simulations of semiconductor materials with focus on their mechanical, magnetic, optical, electronic, and thermal properties. b. Contribution in research projects of the unit. c. Teaching of quantum chemistry package tutorial and simulation techniques to the master students.	School of Mechanical Engineering, University of Tehran (UT), Iran
PhD Research Fellow 10/2015- 3/2019	Department of Chemical Sciences, University of Padova, Italy
R & D Researcher 6/2012- 6/2015	Research and Development Section, Samen Pharmaceutical Company, Iran
Teacher Assistant in Physical Chemistry Laboratory 4/2011- 4/2012	Department of Chemistry, University of Damghan, Iran
Researcher and General	Ghalamchi Educational Organization, Iran

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Chemistry Instructor 10/2006- 8/2010	
Intern and Chemical Expert in Chemistry Laboratory 10/2004- 7/2006	Chemistry Laboratory, Iranian Tobacco Company (ITC), Iran

ISTRUZIONE E FORMAZIONE

Titolo	Corso di studi	Università	anno conseguimento titolo
Laurea Magistrale o equivalente			
Specializzazione			
Dottorato Di Ricerca	Molecular Science	University of Padova	2019
Master	Physical Chemistry	Applied Sciences University of Damghan	2012
Diploma Di Specializzazione Medica			
Diploma Di Specializzazione Europea			
Bachelor	Applied Chemistry	Teacher Training University of Tehran	2004

ISCRIZIONE AD ORDINI PROFESSIONALI

Data iscrizione	Ordine	Città

LINGUE STRANIERE CONOSCIUTE

lingue	livello di conoscenza
Persian	Original Language
English	Advanced
Italian	Intermediate

PREMI, RICONOSCIMENTI E BORSE DI STUDIO

anno	Descrizione premio
2019	Post-Doc Researcher, University of Tehran, Iran
2015	PhD Researcher, University of Padova, Italy
2006	Young Researcher, Ghalamchi educational organization, Iran

ATTIVITÀ DI FORMAZIONE O DI RICERCA

descrizione dell'attività

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ATTIVITÀ PROGETTUALE

2021	Researcher and team member of research project named "Hydrogen Storage Across Length Scales; Hierarchical Hydride-Metal Organic Framework Nanocomposites", University of Glasgow, United Kingdom.
2021	Researcher and team member of research project named "Experimental and Theoretical Study on the Effect of Sm_{3+}, Eu_{3+} and Er_{3+} Substitutions on Crystallite-Size Dependent Properties of $Bi_2Fe_4O_9$", University of Bremen, Germany.
2020	Researcher and team member of research project named "Theory of Vibrational Spectroscopy of Adsorbates at Surfaces", University of Potsdam, Germany.

TITOLARITÀ DI BREVETTI

Brevetto

CONGRESSI, CONVEGNI E SEMINARI

Data	Titolo	Sede
2016	Seminars Towards Enterprise for PhD Students	Confindustria Padova, Italy
2016	Synchrotron Light in Chemical and Life Sciences: Reality and Perspectives	University of Padova, Italy
2016	Space-time Multiscale Approches for Research and Technology	Scuola Normale Superiore, Pisa, Italy

PUBBLICAZIONI

Peer-reviewed:

Mohebbi, E., Seyyed Fakhrabadi, M. M. "Predicting the band gaps of COFs materials by the combination of DFT and machine learning algorithms", Under Working.
Mohebbi, E., Seyyed Fakhrabadi, M. M. "First-principles characterization of honeycomb BeN_2 monolayers: Implications as catalysts for water splitting", Under Submitting.
Mohebbi, E., Seyyed Fakhrabadi, M. M. "Strain-tunable electronic bandgap of black phosphorus-structured nitrogen with desirable optical and elastic properties: A DFT study", Under Review in the Journal of Materials Science & Engineering B.
Mohebbi, E., Seyyed Fakhrabadi, M. M. "Electronic, optical, mechanical, and thermal properties of diphenylacetylene-based graphyne nanosheet using density functional theory", Nanotechnology, DOI: 10.1088/1361-6528/ac0d81, 2021.
Sedona, F., Seyyed Fakhrabadi, M. M., Carlotto, S., Mohebbi, E., Francesco D. B., Casarin, M., Sambi, M. "On-surface synthesis of extended linear graphyne molecular wires by protecting the alkynyl group". Physical Chemistry Chemical Physics, DOI: 10.1039/D0CP01634A, 2020.
Carlotto, S., Mohebbi, E., Sedona, F., Lo Cicero, M., Colazzo, L., Mariani, C., Betti, M. G., Sambi,M. Casarin, M. "An experimental and theoretical study of metallorganic coordination networks of tetrahydroxyquinone on Cu(111)". New Journal of Chemistry, DOI: 10.1039/c9nj04884g, 2019.
Mohebbi, E. "Adsorption of ethylene and acetylene molecules on Ag(110) surface". Journal of

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Nanomaterials & Molecular Nanotechnology, DOI: 10.4172/2324-8777.1000231, 2017.
Mohebbi, E., Ajloo, D. "Quantum mechanical simulation of adenosine deaminase active site". Clinical Biochemistry, DOI: 10.1016/j.clinbiochem.2011.08.240, 2011.

Papers Presented at International Conferences:

Mohebbi, E., Carlotto, S., Sedona, F., Mariani, C., Betti, M. G., Sambi, M., Casarin, M. "Metal–organic coordination networks of tetrahydroxyquinone on Cu(111) based on copper adatom tetramers". Proceedings of the Advanced Inorganic Materials: Green and Unconventional Synthesis Approaches and Functional Assessment (AIM 2018) Conference at Padova, Italy, September 2018.
Mohebbi, E., Carlotto, S., Sedona, F., Mariani, C., Betti, M. G., Sambi, M., Casarin, M. "Metal–organic coordination networks of tetrahydroxyquinone on Cu(111) based on copper adatom tetramers". Proceedings of the 34st European Conference on Surface Science, Aarhus, Denmark, August 2018.
Mohebbi, E., Carlotto, S., Seyyed Fakhrabadi, M. M., Sedona, F., Sambi, M., Casarin, M. "Insight into surface-confined 2D polymerization of a 1,2-bis(4-bromophenyl)ethyne on Ag(110) surface". Proceedings of the 33st European Conference on Surface Science, Szeged, Hungary, August 2017.
Mohebbi, E., Carlotto, S., Seyyed Fakhrabadi, M. M., Sedona, F., Sambi, M., Casarin, M. "Bottom-up synthesized covalent organic nanowires by halogen-based molecules on Ag(110) surface". Proceedings of the 1st European Conference on Chemistry of Two-Dimensional Materials (Chem2DMat), Strasbourg, France, August 2017.
Mohebbi, E., Ajloo, D., "Quantum mechanical simulation of ethylene epoxidation mechanism by tetrafluoro oxo chromate and tetrachloro oxo chromate catalysts". Proceedings of the 15th Iranian Chemistry Congress (ICC) in co-operation with the Iranian Chemical Society (ICS), Mashhad, Iran, September 2011.
Mohebbi, E., Ajloo, D. "Quantum mechanical simulation of adenosine deaminase active site". Proceedings of the 12th Iranian Congress of Biochemistry & 4th International Congress of Biochemistry and Molecular Biology, Mashhad, Iran, September 2011.

ALTRE INFORMAZIONI

TRAINING & COURSES

"Defect Chemistry and Structural Properties of Solids", Jürgen Janek and Wolfgang Zeier, Department of Chemical Science, University of Padova, Italy, 2018.
"The Surface Chemistry of Molecular Monolayers", Francesco Sedona, Department of Chemical Science, University of Padova, Italy, 2017.
"Advanced Inorganic Chemistry and Crystal Field Theory", Maurizio Casarin, Department of Chemical Science, University of Padova, Italy, 2017.
"Quantum Mechanics Concepts and Applications", Mohammad Karimi, Sharif University of Technology, Tehran, Iran, 2015.

HONORS & AWARDS

Best Paper Award from the Journal of Material Chemistry C, 1st European Conference on Chemistry of Two-Dimensional Materials (Chem2DMat), France, 2017.
Encouragement Letter for Being the Most Active Employee in Creativity and Hardworking, Samen Pharmaceutical Company, Iran, 2014.
Best Paper Award, 5th Iranian Chemistry Congress (ICC), Iran, 2011.
Best Researcher Award, Ghalamchi Educational Organization, Iran, 2009.

Ranked "Among Top 1%" in the National Universities Entrance Exam (Konkoor), Iran, 2000.

RESEARCH INTERESTS

Theoretical Chemistry, Quantum Mechanics, Density Functional Theory, Material Sciences, Condensed Matter Physics, Semiconductor Physics and Devices, Nanotechnology, Surface Chemistry, Solid-solid Interfaces, Adsorption/Desorption, Photochemistry and Spectroscopy.

SCIENTIFIC PROGAMMING AND MODELLING

Expert in high throughput simulation and first principles computational modelling.
Experienced in fabrication of different type of materials on metal surfaces such as metallorganic frameworks, covalent organic frameworks, bulk materials, graphene, graphynes, and high-energy-density materials.
Expert In material characterizations such as structural and dynamic stabilities, electronic structure calculations, mechanical behaviour, magnetic and optical properties, phononic and phase transitions, thermal conductions, scanning tunnelling microscopy (STM) and X-ray adsorption spectra simulations.
Expert in developing code within the Quantum Espresso, Phonopy and Phono3py packages, and familiarity with other computational quantum chemistry packages such as Gaussian, VASP and CP2K.
Experience in Bash scripting and common scientific programming languages such as Python and MATLAB, and parallel programming like MPI and OpenMP.
Familiarity with Machine Learning concepts and algorithms, and Python programming experience in libraries such as NumPy, SciPy, Pandas, Matplotlib, StatsModels, Seaborn and ScikitLearn.
Familiarity with some experimental spectroscopic techniques such as low energy electron diffraction (LEED) and X-ray diffraction (XRD).

Le dichiarazioni rese nel presente curriculum sono da ritenersi rilasciate ai sensi degli artt. 46 e 47 del DPR n. 445/2000.

Il presente curriculum, non contiene dati sensibili e dati giudiziari di cui all'art. 4, comma 1, lettere d) ed e) del D.Lgs. 30.6.2003 n. 196.

Luogo e data: _23/08/2021_____, _____

FIRMA___Elaheh Mohebbi_____

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