europass

Miha Gunde

Date of birth: | **Nationality:** | **Gender:**

WORK EXPERIENCE

01/01/2021 - 31/12/2021 - Trieste, Italy
RESEARCH FELLOWSHIP – CONSIGLIO NAZIONALE DELLE RICERCHE - ISTITUTO OFFICINA DEI MATERIALI (CNR-IOM)

Development and application of multi-scale/multi-methods approaches for modelling complex systems, within the research activities of contract between the CNR-IOM and CEA: "Development of an Inter-atomic SMTB-Q for the generation of oxide/semiconductor interface".

09/2017 - 31/12/2020 - Toulouse, France
PHD FELLOWSHIP CONTRACT – MINISTÈRE DE L'ENSEIGNEMENT SUPÉRIEUR ET DE LA RECHERCHE

Development of multiscale computational tools for modelling the evolution of microstructures of materials. Mainly focused on developing shape matching and descriptor algorithms for atomic structures, primarily aimed for use in kinetic Monte Carlo methods, while retaining the generality of approaches to the maximum extent.
The work has been done within the framework of an International Emerging Action (IEA, ex-PICS), ModMicroMat reference 07799, at Laboratoire d'analyse et d'architecture des systèmes (LAAS-CNRS, Toulouse).

EDUCATION AND TRAINING

09/2017 - 26/11/2021 - Toulouse, France
PHD DEGREE IN PHYSICS – Université Paul Sabatier, Toulouse III

Development and implementation of a shape matching algorithm, and its insertion into a general off-lattice kinetic Monte Carlo kernel. The algorithm is needed at the point of recognition and comparison of equivalent local atomic environments. The equivalence is first suggested by isomorphism of simple graphs, and confirmed/rejected by the shape matching. The development and implementation are discussed in detail, and examples of various simulations are shown.
Thesis supervised by: dr. Anne Hemeryck, and dr. Layla Martin-Samos
Online repository link: http://thesesups.ups-tlse.fr/5109/

Thesis: Development of IRA: a shape matching algorithm, its implementation, and utility in a general off-lattice kMC kernel

EQF level 8

10/2018 - 01/2019 - Montréal, Canada
TRAINEESHIP – Université de Montréal

Training on use and coding of kART and ARTn with prof. Normand Mousseau, who is the original author of both codes.

2/5/2022

2014 – 2017 – Nova Gorica, Slovenia

MASTER'S DEGREE IN PHYSICS – University of Nova Gorica

An ab-initio study of three Mg surfaces by means of DFT calculations using Quantum ESPRESSO.
Thesis supervisor: dr. Layla Martin Samos.
Online repository link: http://repozitorij.ung.si/IzpisGradiva.php?id=3134&lang=eng

Thesis: Characterization of Mg low-index surfaces by first-principles

9.33 | EQF level 7 | ECTS | 120

04/2016 – 07/2016 – Trieste, Italy

TRAINEESHIP – University of Trieste and SISSA

with the title "Implementation of semi-empirical van der Waals correction (Grimme-D3)" inside Quantum ESPRESSO, under the supervision of prof. Paolo Giannozzi and prof. Stefano de Gironcoli, within the ERASMUS+ program (April - June 2016) and within the SISSA undergraduate fellowships (July 2016).

09/2014 – 02/2015 – Groningen, Netherlands

STUDY EXCHANGE – Rijksuniversiteit Groningen

One semester study exchange within the ERASMUS+ program.

09/2011 – 08/2014 – Nova Gorica, Slovenia

BACHELOR'S DEGREE IN PHYSICS – University of Nova Gorica

An experimental study of morphology of thin films of P3HT+graphene using the Scanning Electron Miscroscope.
Thesis supervisor: dr. Mattia Fanetti.
Online repository link: http://repozitorij.ung.si/IzpisGradiva.php?id=2182&lang=eng

Thesis: The morphology dependence on growth parameters in nanostructured semiconductors

EQF level 6

LANGUAGE SKILLS

Mother tongue(s): **SLOVENIAN**

Other language(s):

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Spoken production	Spoken interaction	
ENGLISH	C2	C2	C2	C2	C2
FRENCH	B1	B2	B2	B2	B1
ITALIAN	A1	A1	A1	A1	A1

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user

2/5/2022

PUBLICATIONS

Iterative Rotations and Assignments (IRA): A shape matching algorithm for atomic structures

Software Impacts 12, 100264 (2022)
https://doi.org/10.1016/j.simpa.2022.100264 - 2022
Authors: Gunde M, Salles N, Hemeryck A, Martin-Samos L

Activation–Relaxation Technique: An efficient way to find minima and saddle points of potential energy surfaces

Computational Materials Science 209, 15, 111363 (2022)
https://doi.org/10.1016/j.commatsci.2022.111363 - 2022
Authors: Jay A, Gunde M, Salles N, Poberznik M, Martin-Samos L, Richard N, de Gironcoli S, Mousseau N, Hemeryck A

IRA: A Shape Matching Approach for Recognition and Comparison of Generic Atomic Patterns

J. Chem. Inf. Model. 2021, 61, 11, 5446–5457
https://pubs.acs.org/doi/10.1021/acs.jcim.1c00567 - 2021
Authors: Gunde M, Salles N, Hemeryck A, Martin-Samos L

Finding reaction pathways and transition states: r-ARTn and d-ARTn as an efficient and versatile alternative to string approaches

J. Chem. Theory Comput. 2020, 16, 10, 6726–6734
https://pubs.acs.org/doi/10.1021/acs.jctc.0c00541 - 2020
Authors: Jay A, Huet C, Salles N, Gunde M, Martin Samos L, Landa G, Goiffon V, de Gironcoli S, Hemeryck A, Mousseau N

First-principles characterization of Mg low-index surfaces: structure, reconstructions, and surface core-level shifts

Phys. Rev. B 100, 075405 (2019)
https://journals.aps.org/prb/abstract/10.1103/PhysRevB.100.075405 - 2019
Authors: Gunde M, Martin Samos L, de Gironcoli S, Fanetti M, Orlov D, Valant M

CONFERENCES

12/11/2019 - 15/11/2019

Descriptor of a local environment combining topology and geometry, for an atom-resolved off-lattice kMC

Talk at "Progresses and Challenges in Modeling Activated Phenomena: From Machine Learned Energy Surface Sampleing to Multi-Scaling Approaches", November 12-15, 2019, Toulouse, France

07/06/2021 - 11/06/2021

A shape matching algorithm for off-lattice atom-resolved kinetic Monte Carlo

Talk at "Match Chem Comp 2021", June 7-11, Dubrovnik, Croatia (online)

2/5/2022

15/03/2021 – 19/03/2021

An off-lattice kinetic Monte Carlo kernel guided by topological and geometrical analysis to bridge accurate ab-initio calculations and large scale simulations

Talk at "APS March Meeting, March 15-19 2021, online"

05/07/2021 – 09/07/2021

A local-environment descriptor combining topology and geometry, for atom-resolved off-lattice KMC

Poster at "PASC21, July 5-9 2021, Geneva, Switzerland (online)"

JOB-RELATED SKILLS

Software knowledge

Quantum ESPRESSO - software for electronic-structure calculations and materials modeling at the nanoscale, based on density-functional theory (DFT), plane waves, and pseudopotentials:

- implementation of Grimme D3 (dftd3) corrections;
- knowledge of PWscf package;

ARTn - software for the exploration of transition states, or saddle points of a potential energy surface, based on the Lanczos diagonalization and constrained relaxation:

- knowledge of original source code and calculations.

kART - a kinetic Monte Carlo (kMC) software employing ARTn to automatize the exploration of events:

- knowledge of original source code and calculations.

OXCAD - kinetic Monte Carlo for Si surface oxidation modelling:

- knowledge of original source code;

other software:

- lammps (molecular dynamics software for materials modeling);
- ovito (visualization and analysis of output data of particle-based simulations).

Programming languages:
modern Fortran, Python, LaTeX

2/5/2022