



Ismail Can OGUZ

Curriculum Vitae

Personal Information

Nationality French

Date of Birth 14/07/1987

Civil Status Single

Diplomes

Jan 2023– **Master in Data Science**, CentraleSupélec (*Openclassrooms*), Paris.

Dec 2023 *supervised by Stanislas Larnier*

Dec 2014– **Phd in Chemistry**, ENSCM (ICGM-MACS), Montpellier.

Feb 2018 *supervised by Hazar Guesmi*

Chemical order and reactivity of Au-Pd(100) alloy surface: from vacuum to reaction conditions

Sept 2011– **Master of Science in Physics**, Bilkent University, Ankara.

Aug 2013 *supervised by Oğuz Gülsen*

Ab-initio study of iridium on silicon (001) surface

Sept 2006– **Bachelor of Science in Physics**, Bilkent University, Ankara.

June 2011

Professional and Academic Experience

Dec 2023– **Postdoctoral researcher**, DIFFER, Eindhoven, Netherlands.
in collaboration with Suleyman Er

AI-based material discovery for Hydrogen Evolution Reaction (HER) and Oxygen Evolution Reaction (OER)

May 2021– **Postdoctoral researcher**, ENS -LPENS- UMR8023 , Paris, France.
July 2022 *in collaboration with Marie-Laure Bocquet*

The surface affinity of graphene oxide with respect to different organic molecules and adsorption mode search on pristine and graphene oxide

May 2020– **Postdoctoral researcher**, Chimie ParisTech - I-CLEHS- CTM group , Paris, France.
May 2021 *in collaboration with Frédéric Labat*

Software development and Validation within the Generalized Implicit Solvation project, on developing, applying and validating the finite-difference implicit solvation model in the CRYSTAL code

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Oct 2018– Postdoctoral researcher, Université de Montpellier - LabEx CheMISyst, Montpellier,
Nov 2019 France.

in collaboration with Frédéric Jaouen, Tzonka Mineva

Magnetisation in Fe Embedded Porphyrin like Graphene and the Effect of Spin Polarized ZigZag Edges

Publications

- Ismail Can Oguz, Nabil Khossossi, Marco Brunacci, Haldun Bucak, Süleyman Er ***Machine Learning-Accelerated Discovery of Earth-Abundant Bimetallic Electrocatalysts for the Hydrogen Evolution Reaction, ACS Catalysis*** (Accepted, 2025). doi:10.1021/acscatal.5c04967
- Ismail Can Oguz, Frederic Jaouen, and Tzonka Mineva ***Exploring Spin Distribution and Electronic Properties in FeN₄-Graphene Catalysts with Edge Terminations, Molecules*** 29, (2024) 2 : 479
- Dario Vassetti, Ismail Can Oguz, Frédéric Labat, ***Generalizing Continuum Solvation in Crystal to Nonaqueous Solvents: Implementation, Parametrization, and Application to Molecules and Surfaces, Journal of Chemical Theory and Computation*** 17.10 (2021): 6432-6448
- Ismail Can Oguz, Dario Vassetti, Frédéric Labat, ***Assessing the performances of different implicit solvation models for the calculation of hydration energies of molecules, polymers and surfaces: a comparison between the SMD, VASPsol and FDDB models, Theoretical Chemistry Accounts*** 140.8 (2021) 1-13
- Jingkun Li, Moulay Tahar Sougrati, Andrea Zitolo, James Ablett, Ismail Can Oguz, Tzonka Mineva et al., ***Identification of durable and non-durable FeNx sites in Fe-N-C materials for proton exchange membrane fuel cells, Nature Catalysis*** 1-10 (2020)
- Fang Luo, David A. Cullen, Luca Silvioli, Aaron Roy, Moulay Tahar Sougrati, Ismail Can Oguz, Tzonka Mineva et al. ***P-block single-metal-site tin/nitrogen-doped carbon fuel cell cathode catalyst for oxygen reduction reaction*** *Nature Materials* 1-9(2020)
- Ismail Can Oguz, Hazar Guesmi, Dominique Bazin, Frederik Tiemens, ***Predicting the Activity of Nano Transition Metal DeNox Catalysts, J. Phys. Chem. C***, 123, 33, (2019)
- Ismail Can Oguz, Jérôme Creuze, Tzonka Mineva, Hazar Guesmi, ***Equilibrium Au-Pd(100) surface structures under CO pressure : energetic stabilities and phase diagrams, J. Phys. Chem. C***, 122, 33, (2018)
- Ismail Can Oguz, Jérôme Creuze, Tzonka Mineva, Hazar Guesmi, ***The effect of Pd ensemble structure on the O₂ dissociation and CO oxidation mechanisms on Au-Pd(100) surface alloys, J. Chem. Phys.*** 148, 024701 (2018)
- Fatima, Ismail Can Oguz, Deniz Çakır, Sehtab Hossain, Rasika Mohottige, Oguz Gulseren, Nuri Oncel, ***On the structural and electronic properties of Ir-silicide nanowires on Si(001) surface, Journal of Applied Physics*** 120, 095303 (2016)
- Beien Zhu, Ismail Can Oguz, Hazar Guesmi, ***Investigation of finite-size effects in chemical bonding of AuPd nanoalloys, J. Chem. Phys.*** 143, 144309 (2015)
- Ismail Can Oguz, Marie-Laure Bocquet, ***Adsorption Affinities of Organic Molecules on Graphene Oxide from Ab Initio Simulations in Implicit and Explicit Water Solvent, (to be submitted)***

Presentations

- Talks
- *Theoretical Prediction of the Distribution of Spin Moment on Metal-N-C Catalyst Embedded in Truncated Graphene Sheets*, 236th ECS Meeting - October 2019 - Atlanta/USA
 - *Can Density Functional Theory Predict Mössbauer Spectra in Pyrolyzed Fe-N-C Catalysts ?*, 236th ECS Meeting - October 2019 - Atlanta/USA
 - *Spin State Changes in the Zigzag Edge of Graphene Embedded Fe-N-C Catalysts: VASP and deMon2K results*, 19th DeMon2k Developer Workshop - May 2019 - Frejus/France
 - *Pd Segregation on Au-Pd (100) surface and the role of Pd ensembles on the CO oxidation*, JMJC 2017 - October 2017- Montpellier/France
- Posters
- *AI-Driven Bimetal Catalyst Discovery for Green Hydrogen*, NWO Physics 2025 — January 21 2025 — Eindhoven, The Netherlands
 - *AI-Driven Bimetal Catalyst Discovery for Green Hydrogen*, EIREN Energizing Day 2024 — November 19 2024 — Eindhoven, The Netherlands
 - *The effect of graphene truncation on the distribution of spin moment on metal-N-C catalyst : Zig-zag versus armchair edges*, EFCD - September 2019 - La Grande Motte/France
 - *Inverse surface Pd segregation on Pd/Au(001) under CO reactive gas : effect on CO oxidation*, 19th DeMon2k Developer Workshop - May 2019- Frejus/France
 - *Ab initio molecular modelling of bimetallic AuPd (001) surface under reactive CO gas*, PISACMS - August 2016 - Paris/France

Teaching Experience

Bilkent University, Physics Department.

2009–2013 **Recitation Assistant**, Freshmen Physics I-II.

2010 **Teaching Assistant**, Phys 102.

Spring 2012 **Teaching Assistant**, PHYS 316 Electromagnetic Theory II.

Academic Honors and Awards

2006-2011 Bilkent University Board of Trustees Scholarship awarded for undergraduate study

Computer Skills

- Programming & Scripting **Advanced:** PYTHON (including libraries scikit-learn, PyTorch), MATLAB, FORTRAN
Intermediate: SQL
- Scientific Computing **Advanced:** Quantum ESPRESSO, VASP, CP2k, deMon2k, CRYSTAL, XCrySDen, VESTA, Avogadro, Material Studio, VMD, P4Vasp **Software Tools:** Origin9, XMGrace
- Development **Advanced:** LATEX, git **Experienced:** Visual Studio, Jupyter (Kaggle, Colab)
- Data Processing **Intermediate:** Apache Spark

Attended Workshops

GPU Programming 2024, Netherlands eScience Center — Amsterdam (2–3 December 2024)

Young Researcher's Workshop on Machine Learning for Materials Science 2019, Aalto University - Helsinki

19th DeMon2k Developer Workshop 2019, University Paris Saclay - Paris

Paris International School on Advanced Computational Materials 2016, Université Pierre et Marie Curie - Paris

Languages

fluent **English, Turkish (native)**

intermediate **French**

Personal interests

Theatre, Surrealist movies, Running.

References

Tzonka Mineva, ICGM - UMR 5253, Montpellier, FR *tzonka.mineva@enscm.fr*

Hazar Guesmi, ICGM - UMR 5253, Montpellier, FR *hazar.guesmi@enscm.fr*

Frederic Labat, PSL - FRE 2027, Paris, FR *frederic.labat@chimieparistech.psl.eu*

Suleyman Er, DIFFER-Chemical Energy, Eindhoven, NL *s.er@differ.nl*