



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 Gülseren
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 Vasseti, 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 Vasseti, 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 FDPB 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 FeN_x 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 Tielens, *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*, EIRES 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

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|-------------------------|---|
| 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: L ^A T _E X, 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

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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@diffier.nl*