CURRICULUM VITAE

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EDUCATION

- Ph.D. in Computational Chemistry, University of Crete, Greece (2009)
- M.Sc. in Chemistry & Technology of Materials, University of Ioannina, Greece (2008)
- B.Sc. in Materials Science and Engineering, University of Ioannina, Greece (2004)

PROFESSIONAL EXPERIENCE AND APPOINTMENTS

09/2018 – present:	Associate Researcher, Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Greece
03/2017 – 09/2018:	Postdoctoral Research Associate with IKY scholarship, Chemistry Department, University of Crete, Greece
10/2010 – 11/2015:	Postdoctoral Research Associate, Chemistry Department, University of Crete, Greece
11/2009 - 8/2010:	Fuel and Lubricant Quality control, Hellenic Air Force (Military service).

MAIN RESEARCH INTERESTS

- Gas adsorption and separation for energy and environmental applications
- Design of novel Nanostructured and Nanoporous materials with emphasis in Metal-Organic Frameworks and Carbon based systems
- Electronic structure calculations
- Multi-scale computational techniques for gas adsorption
- Calculation of electronic and mechanical properties of 2D heterostructures
- Materials Informatics

EXTERNAL FUNDING

- Hellenic Foundation for Research and Innovation (HFRI), Grand for post-doctoral researchers, GRAFEL, Participant, 2018-present.
- Greek State Scholar Foundation (IKY) Grand for supporting post-doctoral researchers, post-doctoral researcher, 2017-2018.
- General Secretariat for Research and Technology (GSRT), THALES, post-doctoral researcher, 2014-2015.
- General Secretariat for Research and Technology (GSRT), ARISTEIA II, post-doctoral researcher, 2014-2015.
- General Secretariat for Research and Technology (GSRT), COOPERATION, post-doctoral researcher, 2010-2012 and 2013-2014.

TEACHING EXPERIENCE

- Course Instructor (Katsaraki University Scholarship) in the Course "Computational methods applied for studying molecules, nanomaterials and environmental applications", Department of Chemistry, University of Crete, Greece, Spring 2017.
- Course Instructor (ΠΔ 407/80) in the Course "Industrial Chemistry", Department of Chemistry, University of Crete, Greece, Spring 2012.
- Course Instructor (ΠΔ 407/80) in the Course "Computational methods for

studying molecules and nanomaterials", Department of Chemistry, University of Crete, Greece, Spring 2011.

- Course Instructor (ΠΔ 407/80) in the Course "Computational methods for studying molecules and nanomaterials", Department of Chemistry, University of Crete, Greece, Fall 2010.

PROFESSIONAL AFFILIATIONS & ACTIVITIES

- Organizing Committee Member for the International Symposium on advanced nanoporous and nanostrucutred materials, 3–4 September 2014, Heraklion Crete, Greece.
- Organizing Committee Member for the 5th Pan-Hellenic symposium on Porous Materials, University of Crete, 30 June-1st July 2011, Heraklion Crete Greece.
- Member of the Pan-Hellenic Society of Materials Engineers (ΠΑΣΔΜΕΥ).
- Reviewer for scientific research journals in the fields of physical chemistry, materials, and hydrogen economy.

AWARDS AND DISTINCTIONS

- Hellenic Foundation for Research and Innovation (HFRI), Grand for post-doctoral researchers (GRAFEL), as post-Doctoral Researcher, now as Participant, 2018-present.
- Greek State Scholar Foundation (IKY) Grand for supporting post-doctoral researchers (post-Doctoral researcher), 2017-2018.
- Paper "Reticular Synthesis of HKUST-like tbo-MOFs with enhanced CH_4 storage" *J. Am. Chem. Soc.* 2016, 138, 1568-1574 was highlighted in the cover of the corresponding issue.
- Katsaraki University Scholarship for instructing Undergraduate Course at the Department of Chemistry, University of Crete, Greece, Spring 2017.

SELECTED PUBLICATIONS

1. E. Klontzas, A. Mavrandonakis, E. Tylianakis, G. E. Froudakis, "Improving Hydrogen Storage Capacity of MOF by Functionalization of the Organic Linker with Lithium Atoms", *Nano Lett*, 2008, 8, 1572.

2. A. Mavrandonakis, E. Klontzas, E. Tylianakis, G. E. Froudakis, "Enhancement of Hydrogen Adsorption in Metal-Organic Frameworks by the Incorporation of the Sulfonate Group and Li Cations. A Multiscale Computational Study", *J. Am. Chem. Soc.* 2009, 131, 13410.
3. E. Klontzas, E. Tylianakis, G. E. Froudakis, "Design of 3D-COF with enhanced hydrogen storage capacity", *Nano Lett.*, 2010, *10*, 452.
4. E. Klontzas, E. Tylianakis, G.E. Froudakis, "On the Enhancement of Molecular Hydrogen Interactions in Nanoporous Solids for Improved Hydrogen Storage", *J. Phys. Chem. Lett.*, 2011, 2, 1824-1830.
5. T. Lazarides, G. Charalambidis, A. Vuillamy, M. Reglier, E. Klontzas, G. Froudakis, S. Kuhri, D. M. Guldi, A. G. Coutsolelos, "Promising Fast Energy Transfer System via an Easy Synthesis: Bodipy–Porphyrin Dyads Connected via a Cyanuric Chloride Bridge, Their Synthesis and Electrochemical and Photophysical Investigations", *Inorg. Chem.*, 2011, 50, 8926-8936.
6. E. Tylianakis, G. K. Dimitrakakis, F. J. Martin-Martinez, S. Melchor, J. A. Dobado, E. Klontzas, G. E. Froudakis, "Designing novel nanoporous architectures of carbon nanotubes for hydrogen storage" *Int. J. Hyd. Ener.*, 2014, 39, 9825-9829.
7. I. Spanopoulos, C. Tsangarakis, E. Klontzas, E. Tylianakis, G. Froudakis, K. Adil, Y. Belmabkhout, M. Eddaoudi, P. N. Trikalitis, "Reticular Synthesis of HKUST-like tbo-MOFs with enhanced CH_4 storage" *J. Am. Chem. Soc.* 2016, 138, 1568-1574.
8. M. G. Frysali, E. Klontzas, E. Tylianakis, G. E. Froudakis, "Tuning the interaction strength and the adsorption of CO_2 in metal-organic frameworks by functionalization of the organic linkers" *Micro. Meso. Mat.* 2016, 227, 144-151.
9. I. Spanopoulos, C. Tsangarakis, S. Barnett, H. Nowell, E. Klontzas, G. E. Froudakis, P. N. Trikalitis, "Directed assembly of a high surface area 2D metal–organic framework displaying the augmented "kagomı dual" (kgd-a) layered topology with high H_2 and CO_2 uptake" *Inorg. Chem. Front.* 2017, 4, 825-832.
10. M. Kotzabasaki, I. Galdadas, E. Tylianakis, E. Klontzas, Z. Cournia, G. E. Froudakis, "Multiscale simulations reveal IRMOF-74-III as a potent drug carrier for gemcitabine delivery" *J. Mat. Chem. B* 2017, 5, 3277-3282.
11. G. Borboudakis, T. Stergiannakos, M. Frysali, E. Klontzas, I. Tsamardinos, G. E. Froudakis, "Chemically intuited, large-scale screening of MOFs by machine

learning techniques" *npj Computational Materials* 2017, 3, 40.

12. G. S. Fanourgakis, K. Gkagkas, E. Tylianakis, E. Klontzas, G. E. Froudakis, "A Robust Machine Learning Algorithm for the Prediction of Methane Adsorption in Nanoporous Materials", *J. Phys. Chem. A* 2019, Accepted, DOI: 10.1021/acs.jpca.9b03290.
13. L. P. Zârbo, M. A. Oancea, E. Klontzas, E. Tylianakis, I. G. Grosu, G. E. Froudakis, "Electrically Enhanced Hydrogen Adsorption in Metal-Organic Frameworks", *ChemRxiv* 2019, doi.org/10.26434/chemrxiv.8209304.v1.
14. E. Klontzas, G. E. Froudakis I. Skarmoutsos, K. Galiotis, E. N. Koukaras, "Structural, Electronic and Mechanical Properties of Molecularly Pillared, 3D Nanoporous Graphene Materials", *conference proceedings*, 12th Panhellenic Scientific Conference of Chemical Engineering 2019.
15. E. Klontzas, E. Tylianakis, V. Varshney, A. K. Roy, G. E. Froudakis, "Organically interconnected graphene flakes: A flexible 3-D material with tunable electronic bandgap", *Nature Scientific Reports* 2019, accepted, reference number: SREP-17-48832C.