

## CURRICULUM VITAE

### EMMANUEL KLONTZAS

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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 (ΠΑΔ 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 nanostructured 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<sub>4</sub> 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. Tylanakis, 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<sub>4</sub> storage" *J. Am. Chem. Soc.* 2016, 138, 1568-1574.
8. M. G. Frysalis, E. Klontzas, E. Tylianakis, G. E. Froudakis, "Tuning the interaction strength and the adsorption of CO<sub>2</sub> 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<sub>2</sub> and CO<sub>2</sub> 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. Frysalis, 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](https://doi.org/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](https://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*, 12<sup>th</sup> 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.