

Emmanuel Klontzas

List of Publications

A. In peer review journals

1. K. Litina, A. Miriouni, D. Gournis, M. A. Karakassides, N. Georgiou, E. Klontzas, E. Ntoukas, A. Avgeropoulos, "Nanocomposites of polystyrene-b-polyisoprene copolymer with layered silicates and carbon nanotubes", *European Polymer Journal* 2006, 42, 2098.
2. E. Klontzas, A. Mavrandonakis, G.E. Froudakis, Y. Carissan and W. Klopper, "Molecular Hydrogen Interaction with IRMOF-1: A Multiscale Theoretical Study", *J. Phys. Chem. C* 2007, 111, 13635.
3. E. Klontzas, E. Tylianakis, G.E. Froudakis, "Hydrogen Storage in 3D Covalent Organic Frameworks. A Multiscale Theoretical Investigation" *J. Phys. Chem. C* 2008, 112, 9095.
4. 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.
5. E. Tylianakis, E. Klontzas, G.E. Froudakis, "The effect of structural and energetic parameters of MOFs and COFs towards the improvement of their hydrogen storage properties", *Nanotechnology* 2009, 20, 204030.
6. 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.
7. E. Klontzas, E. Tylianakis, G.E. Froudakis, "Hydrogen Storage in Lithium-Functionalized 3-D Covalent-Organic Framework Materials" *J. Phys. Chem. C* 2009, 113, 21253.
8. E. Klontzas, E. Tylianakis, G.E. Froudakis, "Design of 3D-COF with enhanced hydrogen storage capacity", *Nano Lett.* 2010, 10, 452.
9. S. Voutsadaki, G.K. Tsikalas, E. Klontzas, G.E. Froudakis, H. E. Katerinopoulos, "A "turn-on" coumarin-based fluorescent sensor with high selectivity for mercury ions in aqueous media", *Chem. Commun.* 2010, 46, 3292.
10. T. Stergiannakos, E. Tylianakis, E. Klontzas, G.E. Froudakis, "Enhancement of Hydrogen adsorption in Metal-Organic Frameworks by Mg+2 Functionalization: A Multiscale Computational Study", *J. Phys. Chem. C* 2010, 114, 16855.
11. E. Tylianakis, E. Klontzas, G.E. Froudakis, "Multi-scale theoretical investigation of hydrogen storage in covalent organic frameworks", *Nanoscale* 2011, 3, 856.
12. 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.
13. 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.
14. T. Stergiannakos, E. Tylianakis, E. Klontzas, P. Trikalitis, G. E. Froudakis, "Hydrogen Storage in Novel Li-doped Corrole Metal-Organic Frameworks", *J. Phys. Chem. C* 2012, 116, 8359-8363.
15. S. Voutsadaki, G.K. Tsikalas, E. Klontzas, G.E. Froudakis, S. A. Pergantis, K. D. Dimadis, H. E. Katerinopoulos, " A cyclam-type "turn-on" fluorescent sensor selective for mercury ions in

aqueous media”, RSC Adv. 2012, 2, 12679.

16. C. – Y. Wang, J. L. Gray, Q. Gong, Y. Zhao, J. Li, E. Klontzas, G. Psfogiannakis, G. Froudakis, A. D. Lueking, “Hydrogen Storage with Spectroscopic Identification of Chemisorption Sites in Cu-TDPAT via Spillover from a Pt/Activated Carbon Catalyst”, J. Phys. Chem. C 2014, 118, 2650-26763.
17. G.K. Tsikalas, P. Lazarou, E. Klontzas, S. A. Pergantis, I. Spanopoulos, P. N. Trikalitis, G.E. Froudakis, H. E. Katerinopoulos, “ A “turn-on” turning-to-ratiometric sensor for Zn(II) ions in aqueous media”, RSC Adv. 2014, 4, 693.
18. P. Xydias, I. Spanopoulos, E. Klontzas, G. E. Froudakis, P. N. Trikalitis, “Drastic enhancement of the CO₂ adsorption properties in sulfone-functionalized Zr- and Hf-UiO-67 MOFs with Hierarchical Mesopores”, Inorg. Chem. 2014, 53, 679.
19. G.N. Kalantzopoulos, A. Enotiadis, E. Maccallini, M. Antoniou, K. Dimos, A. Policicchio, E. Klontzas, E. Tylianakis, V. Binas, P.N. Trikalitis, R.G. Agostino, D. Gourmis, G.E. Froudakis, “Hydrogen storage in ordered and disordered phenylene-bridged mesoporous organosilicas”, Int. J. Hydrogen energy 2014, 39, 2104.
20. M. G. Frysalis, E. Klontzas, G. E. Froudakis, “Ab initio study of the adsorption of CO₂ on functionalized benzenes”, ChemPhysChem 2014, 15, 905.
21. 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. Hydrogen Energy 2014, 39, 9825-9829.
22. T. Stergiannakos, E. Klontzas, E. Tylianakis, G.E. Froudakis, “Enhancement of CO₂ adsorption in Magnesium Alkoxide IRMOF-10” J. Phys. Chem. C 2015, 119, 22001-22007.
23. 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 CH₄ storage” J. Am. Chem. Soc. 2016 138, 1568-1574.
24. D. P. Broom, C. J. Webb, K. E. Hurst, P. A. Parilla, T. Gennett, C. M. Brown, R. Zacharia, E. Tylianakis, E. Klontzas, G. E. Froudakis, Th. A. Steriotis, P. N. Trikalitis, D. L. Anton, B. Hardy , D. Tamburello, C. Corgnale, B. A. van Hassel, D. Cossement, R. Chahine, M. Hirscher, “Outlook and challenges for hydrogen storage in nanoporous materials” Appl. Phys. A 2016, 122:151.
25. M. G. Frysalis, E. Klontzas, E. Tylianakis, G. E. Froudakis, “Tuning the interaction strength and the adsorption of CO₂ in metal-organic frameworks by functionalization of the organic linkers” Micro. Meso. Mat. 2016, 227, 144-151.
26. I. Spanopoulos, I. Bratsos, C. Tampaxis, D. Vourloumis, E. Klontzas, G. Froudakis, G. C. Charalambopoulou, T. A. Steriotis, P. N. Trikalitis, “Exceptional Gravimetric and Volumetric CO₂ Uptake in a Palladated NbO-type MOF Utilizing Cooperative Acidic and Basic, Metal-CO₂ Interactions” Chem. Comm. 2016, 10559-10562.
27. P. Glodic, C. Michesan, E. Klontzas, M. Velegrakis, “Formation, Fragmentation, and Structures of Y_xO_y+ (x = 1, 2, y = 1 – 13) Clusters: Collision-Induced Dissociation Experiments and Density Functional Theory Calculations” J. Phys. Chem. A 2016, 120, 972-980.
28. 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 “kagomé dual” (kgd-a) layered topology with high H₂ and CO₂ uptake” Inorg. Chem. Front. 2017, 4, 825-832.
29. 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.

30. S. Carneado, J. F. Lopez-Sanchez, A. Sahuquillo, E. Klontzas, G. E. Froudakis, S. A. Pergantis, "Antimony speciation in spirits stored in PET bottles: identification of a novel antimony complex" *J. Anal. At. Spectrom.* 2017, 32, 1109-1118.
31. M. Kotzabasaki, E. Tylianakis, E. Klontzas, G. E. Froudakis, "OH-functionalization strategy in Metal-Organic frameworks for drug delivery" *Chem. Phys. Lett.* 2017, 685, 114-118.
32. 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.
33. G. Angeli, C. Sartsidou, S. Vlachaki, I. Spanopoulos, C. Tsangarakis, A. Kourtellaris, E. Klontzas, G. E. Froudakis, A. Tasiopoulos, P.N. Trikalitis, "Reticular Chemistry and the Discovery of a New Family of Rare Earth (4,8)-Connected Metal-Organic Frameworks with csq Topology Based on $\text{Re}_4(\mu_3\text{-O})_2(\text{COO})_8$ clusters" *ACS Appl. Mater. Interfaces* 2017, 9, 44560-44566.
34. 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.
35. 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.

B. Proceedings in Conferences

1. 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.
2. E. Tylianakis, E. Klontzas, G. K. Dimitrakakis, G. E. Froudakis, " Gas adsorption and separation by employing Grand Canonical Monte Carlo simulations", *Computational Methods in Science and Engineering*, vol 2: Advances in Computational Science, AIP Conf. Proc. 2009, 1148, 392.
3. E. Klontzas, G. E. Froudakis, "First Principles Theoretical Study of the Interaction of Hydrogen with the Ultra-Microporous materials IRMOF and COF", *Computational Methods in Science and Engineering*, vol 2: Advances in Computational Science, AIP Conf. Proc. 2009, 1148, 394.

C. Preprints

1. 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.