TPCI (ΙΘΦΧ) 2020

1. Papers in Refereed Journals

1. "Porous carbon nanotube networks and pillared graphene materials exhibiting high SF_6 adsorption uptake and separation selectivity of SF_6/N_2 fluid mixtures: A comparative molecular simulation study",
I. Skarmoutsos, E.N. Koukaras, C. Galiotis, G.E. Froudakis, and E. Klontzas,
Micropor. Mesopor. Mater. 307, 110464 (2020).
DOI: 10.1016/j.micromeso.2020.110464

2. "Confinement effects on the properties of polar hydrogen-bonded fluids: A showcase on methanol adsorbed in three-dimensional pillared graphene and carbon nanotube networks",
I. Skarmoutsos, E.N. Koukaras, G.E. Froudakis, G. Maurin, and E. Klontzas,
J. Phys. Chem. C 124, 22959 (2020).
DOI: 10.1021/acs.jpcc.0c06289

3. "An automated machine learning architecture for the accelerated prediction of metal-organic frameworks performance in energy and environmental applications",
I. Tsamardinos, G.S. Fanourgakis, E. Greasidou, E. Klontzas, K. Gkagkas, and G.E. Froudakis,
Micropor. Mesopor. Mater. 300, 110160 (2020).
DOI: 10.1016/j.micromeso.2020.110160

4. "Hydration structure and dynamics of the favipiravir antiviral drug: A molecular modelling approach",
I. Skarmoutsos, G. Maurin, E. Guardia, and J. Samios,
B. Chem. Soc. Jpn. 93, 1378-1385 (2020).
DOI: 10.1246/bcsj.20200163

5. "Solvation structure and dynamics of the dimethylammonium cation diluted in liquid water: A molecular dynamics approach",
I. Skarmoutsos, E. Guardia,
J. Chem. Phys. 152, 234501 (2020).
DOI: 10.1063/5.0004204

6. "Enhanced organic and perovskite solar cell performance through modification of the electron-selective contact with a bodipy-porphyrin dyad",
K. Gkini, A. Verykios, N. Balis, A. Kaltzoglou, M. Papadakis, K. S. Adamis, K.-K. Armadorou, A. Soultati, C. Drivas, S. Gardelis, I.D. Petsalakis, L.C. Palilis, A. Fakharuddin, M.I. Heider, X. Bao, S. Kennou, P. Argitis, L. Schmidt-Mende, A. G. Coutsolelos, P. Falaras, and M. Vasilopoulou,
ACS Appl. Mater. Inter., 12, 1120 (2020).
DOI: 10.1021/acsami.9b17580

7. “The solvent effect on a styryl-bodipy derivative functioning as an AND molecular logic gate”,
D. Tzeli, I.D. Petsalakis, and G. Theodorakopoulos,
Int. J. Quantum Chem. 120, e26181 (2020).
DOI: 10.1002/qua.26181

8. “Chalcogen bonding and hydrophobic effects force molecules into small spaces”,
F.-U. Rahman, D. Tzeli, I. Petsalakis, G. Theodorakopoulos, P. Ballester, J. Rebek, Jr., and Y. Yu,
J. Am. Chem. Soc. 135, 5876 (2020).
DOI: 10.1021/jacs.0c01290

9. “Binding selectivity and separation of p-functionalized toluenes with a metallo-cavitand in water”,
F.-U. Rahman, J.M. Yang, Y.H. Wan, H.-B. Zhang, I.D. Petsalakis, G. Theodorakopoulos, J. Rebek, and Y. Yu,
Chem. Commun. 56, 6945 (2020).
DOI: 10.1039/d0cc02778b

10. “Aromaticity and chemical bonding of chalcogen-bonded capsules featuring enhanced magnetic anisotropy”,
D. Tzeli, I.D. Petsalakis, G. Theodorakopoulos, F.-U. Rahman, P. Ballester, J. Rebek, Jr., and Y. Yu,
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DOI: 10.1002/cphc.202000654

11. “Suppressing the photocatalytic activity of zinc oxide electron-transport layer in nonfullerene organic solar cells with a pyrene-bodipy interlayer”,
A. Soultati, A. Verykios, S. Panagiotakis, K.-K. Armadorou, M.I. Haider, A. Kaltzoglou, C. Drivas, A. Fakharuddin, X. Bao, C. Yang, A. R. bin M. Yusoff, E. K. Evangelou, I.D. Petsalakis, S. Kennou, P. Falaras, K. Yannakopoulou, G. Pistolis, P. Argitis, and M. Vasilopoulou,
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12. “Quadruple bonding in the ground and low-lying excited states of the diatomic molecules TcN, RuC, RhB, and PdBe”,
D. Tzeli, I.N. Karapetsas,
J. Phys. Chem. A 124, 6667 (2020).
DOI: 10.1021/acs.jpca.0c03208

13. “Reactivity and mechanism of photo- and electrocatalytic hydrogen evolution by a diimine copper(I) complex”,
M. Drosou, F. Kamatsos, G. Ioannidis, A. Zarkadoulas, C. Mitsopoulou, C. Papatriantafyllopoulou, and D. Tzeli,
Catalysts 10, 1302 (2020).
DOI: 10.3390/catal10111302

14. “Electronic properties of the $Sn_{1-x}Pb_xO$ alloy and band alignment of the SnO/PbO system: a DFT study”,
N. Kelaidis, S. Bousiadi, M. Zervos, A. Chroneos, and N.N. Lathiotakis,
Sci. Rep. 10, 16828 (2020).
DOI: 10.1038/s41598-020-73703-y

15. “Density-inversion method for the Kohn-Sham potential: role of the screening density”,
T.J. Callow, N.N. Lathiotakis, and N.I. Gidopoulos,
J. Chem. Phys. 152, 164114 (2020).
DOI: 10.1063/5.0005781

16. “Improving the exchange and correlation potential in density-functional approximations through constraints”,
T.J. Callow, B.J. Pearce, T. Pitts, N.N. Lathiotakis, M.J.P. Hodgson, and N.I. Gidopoulos,
Faraday Discuss. 224, 126 (2020).
DOI: 10.1039/d0fd00069h

17. “Atomic structure and electronic properties of hydrogenated X (=C, Si, Ge, and Sn) doped TiO_2: A theoretical perspective”,
P.-P. Filippatos, N. Kelaidis, M. Vasilopoulou, D. Davazoglou, and A. Chroneos,
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18. “Ultrafast time delay as a control parameter in resonant ionization by two XUV ultrashort pulses”,
Th. Mercouris, Y. Komninos, and C.A. Nicolaides,
J. Phys. B - At. Mol. Opt. 53, 095603 (2020).
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19. “Excitation of superpositions of resonances by two time-delayed ultrafast pulses: Multistate semi-analytic formalism and application to inner-hole states of carbon at the K-absorption edge”,
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O.L.G. Alderman, C.J. Benmore, S. Feller, E.I. Kamitsos, E.D. Simandiras, D.G. Liakos, M. Jesuit, M. Boyd, M. Packard, and R. Weber,
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A.G. Papadopoulos, N.S. Tagiara, E.D. Simandiras, and E.I. Kamitsos,
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N. Sawangboon, A. Nizamutdinova, T. Uesbeck, R. Limbach, E. Meechoowas, K. Tapasa, D. Möncke, L. Wondraczek, E.I. Kamitsos, L. van Wüllen, and D. Brauer,
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23. “Spectroscopic study of the role of alkaline earth oxides in mixed borate glasses - site basicity, polarizability and glass structure”,
H. Othman, H. Elkholy, M.R. Cicconi, D. Palles, D. de Ligny, E.I. Kamitsos, and D. Möncke,
J. Non-Cryst. Solids 533, 119892 (2020).
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24. “Calcium modified clinoptilolite as a recovery medium of phosphate and potassium from anaerobically digested olive mill wastewater”,
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A.G. Kontos, G.K. Manolis, A. Kaltzoglou, D. Palles, E.I. Kamitsos, M.G. Kanatzidis, and P. Falaras,
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K.I. Chatzipanagis, N.S. Tagiara, D. Möncke, S. Kundu, A.C.M. Rodrigues, and E.I. Kamitsos,
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35. "Pyrene coating transition metal disulfides as protection from photooxidation and environmental ageing",
R. Canton-Vitoria, Y. Sayed-Ahmad-Baraza, B. Humbert, R. Arenal, C.P. Ewels, and N. Tagmatarchis,
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M.M. Elsenety, M. Antoniadou, N. Balis, A. Kaltzoglou, L. Sygellou, A. Stergiou, N. Tagmatarchis, and P. Falaras,
ACS Appl. Energy Mater. 3, 2455 (2020).
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38. "In-situ growth and immobilization of CdS nanoparticles onto functionalized MoS_2: preparation, characterization and fabrication of photoelectrochemical cell",
A. Kagkoura, J. Hernandez-Ferrer, A. M. Benito, W. K. Maser, and N. Tagmatarchis,
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A. Kagkoura, R. Canton-Vitoria, L. Vallan, J. Hernandez-Ferrer, A. M. Benito, W. K. Maser, R. Arenal, and N. Tagmatarchis,
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G. Rotas, M.B. Thomas, R. Canton-Vitoria, F. D'Souza, and N. Tagmatarchis,
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N. Martin, N. Tagmatarchis, Q. H. Wang, and X. Zhang,
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I.K. Sideri, R. Arenal, and N. Tagmatarchis,
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M. Elsenety, A. Stergiou, L. Sygellou, N. Tagmatarchis, N. Balis, and P. Falaras,
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46. “Solution-phase molecular recognition of an azafullerene-quinoline dyad by a face-to-face porphyrin-dimer tweezer”,
A. Stergiou, A.K. Andreopoulou, J.K. Kallitsis, and N. Tagmatarchis,
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S. Nufer, P.J. Lynch, M.J. Large, S.P. Ogilvie, J.P. Salvage, M. Pelaez-Fernandez, T. Waters, I. Jurewicz, E. Munoz, R. Arenal, A.M. Benito, W.K. Maser, N. Tagmatarchis, C. Ewels, A. Brunton, and A.B. Dalton,
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R. Canton-Vitoria, S. Nufer, X. Che, Y. Sayed-Ahmad-Baraza, R. Arenal, C. Bittencourt, A. Brunton, A. Dalton, C.P. Ewels, and N. Tagmatarchis,
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N. Naziris, F. Saitta, V. Chrysostomou, M. Libera, B. Trzebicka, D. Fessas, S. Pispas, and C. Demetzos,
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62. "Physicochemical, morphological and thermal evaluation of lyotropic lipidic liquid crystalline nanoparticles: The effect of stimuli-responsive polymeric stabilizer",
M. Chountoulesi, D.R. Perinelli, N. Pippa, V. Chrysostomou, A. Forys, L. Otulakowski, G. Bonacucina, B. Trzebicka, S. Pispas, and C. Demetzos,
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R.K. Raya, M. Stepanek, Z. Limpouchova, K. Prochazka, M. Svoboda, M. Lisal, E. Pavlova, A. Skandalis, and S. Pispas,
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2. Papers in Proceedings of International and National Conferences

1. "Density functional calculations with lattice relaxation of field emitted currents",
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33rd International Vacuum Nanoelectronics Conference (IVNC), Lyon, France, July 6-10, 2020, IEEE Proceedings, pp. 1-2 (2020).

2. "Analysis of physical and structural properties of alkali oxide-modified tellurite glasses",
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4. "Functional surfaces of laser-microstructured silicon coated with polymer blends switching between hydrophilicity and hydrophobicity",
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3. Book Chapters

1. "If truncated wave functions of excited state energy saddle points are computed as energy minima, where is the saddle point?"
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3. "Functionalized carbon nanohorns as drug delivery platforms",
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6. "Dynamics and physics of integrin activation in tumor cells by nano-sized extracellular ligands and electromagnetic fields",
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4. Books Authored

1. Dynamics and applications of photon-nanostructured systems",
E. Sarantopoulou,
Nanomaterials (2020).
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5. Dissertations

a. PhD theses

1. "Development and applications of hybrid nanomaterials and nanostructured surfaces",
M. Kanidi,
Supervisor: Dr. M. Kandyla, University of Patras, Department of Material Science (2020).

2. "Theoretical study and development of photonic devices and sensors",
A. Petropoulou,
Supervisor: Dr. C. Riziotis, University of Peloponnese, Department of Informatics and Telecommunications (2020).

b. MSc theses

1. "On the structure of lithium and strontium borate glasses modified with yttrium and rare-earth cations investigated by vibrational spectroscopy",
B. Topper,
Supervisor: Professor D. Möncke, Inamori School of Engineering, New York State College of Ceramics, Alfred University, NY, USA, and E.I. Kamitsos, TPCI / National Hellenic Research Foundation (11/2020).

2. "Intercalation phenomena in kaolinite: New insights by vibrational spectroscopy",
F. Andreou,
Supervisor: Dr. G.D. Chryssikos, National Technical University of Athens, School of Applied Mathematical and Physical Sciences (2020).
http://dx.doi.org/10.26240/heal.ntua.19974

3. "Preparation and physicochemical characterization of perovskite / polymer hybrid materials",
P. Panagopoulou,
Supervisor: Dr. G. Mousdis, National Technical University of Athens, School of Chemical Engineering (2020).

4. "Amphiphilic P(MMA-co-HPMA)-b-POEGMA block copolymers: Synthesis, characterization, self-assembly in aqueous solutions and encapsulation of drugs",
D. Selianitis,
Supervisor: Dr. S. Pispas, National and Kapodistrian University of Athens, Department of Chemistry (2020).

5. "pH-responsive P(POEGMA-co-DIPAEMA) random copolymers: Synthesis, characterization, self-assembly in aqueous solutions and drug encapsulation",
C. Philippidis,
Supervisor: Dr. S. Pispas, National and Kapodistrian University of Athens, Department of Chemistry (2020).

c. Honors theses

1. "N-confused porphyrins – Ni-Complexes of N-confused tetraphenylporphyrin",
K. Gonianaki,
Supervisor: Dr. D. Tzeli, National and Kapodistrian University of Athens, Department of Chemistry (2020).

d. Internships

1. "On the structure of lithium and strontium borate glasses modified with yttrium and rare-earth cations investigated by vibrational spectroscopy",
B. Topper,
Supervisors: Dr. E.I. Kamitsos, TPCI / National Hellenic Research Foundation and Prof. D. Möncke, Inamori School of Engineering, New York State College of Ceramics, Alfred University, NY, USA (January and February 2020).

2. "Synthèse et caractérisation physicochimique d'un nouveau composé hybride à base d'antimoine",
Tlili Imen,
Supervisors: Dr. G. Mousdis, La Faculté des Sciences de Sfax, Sfax University (2020).

3. "Modification of rheological and physicochemical properties of biopolymer fluids by inclusion of metallic nanoparticles",
A. Saltas,
Supervisor: Dr. A. Papagiannopoulos, National Technical University of Athens, School of Mining and Metallourgical Engineering (2020).

4. "Nanoparticle production based on proteins",
A. Sklapani,
Supervisor: Dr. A. Papagiannopoulos, National Technical University of Athens, School of Applied Mathematical and Physical Sciences (2020).

6. Conference Presentations

1. "DFT study of the photophysical processes of bodipy derivatives eliciting molecular logic gate response",
D. Tzeli, I.D. Petsalakis, G. Theodorakopoulos,
New horizons in density functional theory; Faraday Discussion, Faraday Division of the Royal Society of Chemistry, Online Conference, September 2-4, 2020 (poster).

2. "Graphene based membranes for gas separation: A theoretical study",
N.N. Lathiotakis,
IESL Seminar, IESL/FORTH, Heraklion Crete, December 2, 2020 (invited talk).

3. “Calculating the energy barriers for molecular permeation through sub-nanometer size pores in graphene”,
N.N. Lathiotakis,
Online workshop on Computational Materials Science, Department of Materials Science and Technology, University of Crete, and Hellenic Society for the Science and Technology of Condensed Matter, December 19-20, 2020 (invited talk).

4. “Synthesis and characterization of multilayered ZnO/glass/ZnO varistors”,
C.P.E. Varsamis, C. Valvi*, N. Makris, and E.I. Kamitsos,
International Conference on Technologies and Materials for Renewable Energy, Environment and Sustainability (TMREES20), Athens - Greece, June 25-27, 2020 (oral).

5. “Covalent functionalization of exfoliated MoS_2 with organic motifs for the selective recognition of ions and molecules”,
A. Stergiou*, C. E. Stangel, and N. Tagmatarchis,
17th International Conference on Nanoscience & Nanotechnologies (NN20), Thessaloniki, Greece, 7-10/7/2020 (invited).

6. “Ionic liquid modified MoS_2 sheets for energy conversion application”,
D. K. Perivoliotis*, C. Stangel, and N. Tagmatarchis,
NanoteC20 – Carbon Nanoscience and Nanotechnology, Virtual Meeting, Surrey, UK, 25/8/2020 (e-poster).

7. “Sulfur-doped carbon nanohorns for hydrogen evolution and oxygen reduction reaction”,
A. Kagkoura*, and N. Tagmatarchis,
NanoteC20 – Carbon Nanoscience and Nanotechnology, Virtual Meeting, Surrey, UK, 25/8/2020 (e-poster).

8. “Novel amphiphilic cationic block copolymers by RAFT and their complexes with DNA”,
S. Pispas*,
1st Virtual European Polymer Conference, https://sfill225.wixsite.com/polymerconference, Abo Akademi University, Finland, 17-18/9/2020 (invited talk).

9. “Dehydration process of thermoresponsive molecular brushes with copolymer side chains”,
J.-J. Kan*, J. Zhao, L. C. Barnsley, F. Kohler, H. Dietz, S. Pispas, and C.M. Papadakis,
DPG-Frühjahrstagung (DPG Spring Meeting), Dresden, Germany, 15-20/3/2020 (oral).

10. “Polymer block length and temperature effects on the nanoscale morphology of thermoresponsive double hydrophilic block copolymers”,
A. Vagias*, A. Papagiannopoulos, L.P. Kreuzer, D. Giaouzi, S. Busch, S. Pispas, and P. Müller-Buschbaum,
MLZ User Meeting and German Neutron Scattering Conference,
https://indico.frm2.tum.de/event/225/, Munich, Germany, 8-10/12/2020 (poster).

11. “Multilayers of chitosan-fibrinogen and their effect on cardiac tissue engineering”,
M. Kitsara*, A. Papagiannopoulos, G. Tassis, A. Simon, O. Agbulut, and S. Pispas,
11th World Biomaterials Conference (WBC2020), https://wbc2020.org/, 11-15/12/2020 (poster).

12. “Functional surfaces of laser-microstructured silicon coated with polymer blends switching between hydrophilicity and hydrophobicity”,
M. Kanidi, A. Papagiannopoulos, A. Matei, M. Dinescu, S. Pispas, and M. Kandyla*,
Conference on Lasers and Electro-Optics (CLEO), https://www.cleoconference.org/home/, San Jose, CA USA, 5-2020 (oral).

13. “Polysaccharide/protein nanoparticles by biocompatible methods for the encapsulation of bioactive compounds”,
A. Papagiannopoulos*,
International Webinar on Polymers, Plastics and Composites, 21-22/10/2020 (invited oral).

14. “Formation of nanoparticles from ethanol-denatured whey proteins”,
T. Sentoukas*, G. Charitou, J. Wagner, T. Moschakis, and A. Papagiannopoulos,
ISEKI-e-conference on "Food Quality and Texture in Sustainable Production and Healthy Consumption", https://www.iseki-food.net/events/iseki-e-conference-food-quality-and-texture-sustainable-production-and-healthy-consumption, 18-19/11/2020 (oral).

15. “Photon-processed nanocavity networks regulate a thermodynamic-chaotic state interplay in 2D surfaces”,
V. Gavriil*, A.C. Cefalas, D. Christofilos, G. Kourouklis, Z. Kollia, and E. Sarantopoulou,
Conference on Complex Systems 2020, Thessaloniki, Greece, December 4-11, 2020 (oral).

16. “The hypothesis of quantum coherent brain dynamics and human behavior,
A.C. Cefalas*, V. Gavriil, Z. Kollia, and E. Sarantopoulou,
Conference on Complex Systems 2020, Thessaloniki, Greece, December 4-11, 2020 (oral).

7. Popular Conference Presentations

1. “Χρήση της νανοτεχνολογίας για περισσότερο εύγευστο, υγιεινό και θρεπτικό φαγητό”,
Α. Παπαγιαννόπουλος,
Λαϊκό Πανεπιστήμιο, Διαλέξεις Χειμερινού Εξαμήνου 2020-2021, Αθήνα, Ελλάδα; Οκτώβρης 2020.