Curriculum Vitae

Personal information

Name: George (Yorgos) Volonakis
Date of birth: 5 November 1982
Nationality: French / Greek

ORCID: 0000-0003-3047-2298
Website: http://george-volonakis.univ-rennes.fr
Google Scholar: http://scholar.google.com/citations?user=Viti3pwAAAAJ

Current position

Junior Professor, Université de Rennes — Since September 2022
Insitut des Sciences Chimiques de Rennes, Rennes, FR

Former appointments

Chaire de Recherche Rennes Metropole — January 2020 - August 2022
Insitut des Sciences Chimiques de Rennes, Univerisité de Rennes 1, Rennes, FR

Postdoctoral Research Fellow — April 2014 - December 2019
Materials modelling and design group, Department of Materials, University of Oxford, UK
PI: Prof. Feliciano Giustino.

Education

- Habilitation à diriger des recherches in Chemistry/Physics, — May 2023
  Université de Rennes, Rennes, FR
- PhD in Physics, — February 2014
  Department of Physics, Aristotle University of Thessaloniki, Thessaloniki, GR
  Supervisor: Prof. Stergios Logothetidis. Advisor: Prof. Leonidas Tsetseris
- MSc in Nanosciences and Nanotechnologies — November 2008
  Interdisciplinary and Interdepartmental Postgraduade Program, Department of Physics, Aristotle University of Thessaloniki, GR
  Thesis supervisor: Prof. Stergios Logothetidis.
- BSc in Physics — September 2006
  Department of Physics, Aristotle University of Thessaloniki, GR
  Thesis supervisor: Prof. Stergios Logothetidis: Advisor: Prof. Milan Damnjanovic

Teaching Activities

- First year MSc (Master 1) course and tutorials on Quantum Chemistry, International MSc program Mamaself, Université de Rennes, 2022-2023.
- First year BSc (License 1) tutorials on 'Thermodynamics', Chemistry, Université de Rennes, 2022-2023.

- Third year BSc (License 3) hands-on sessions on 'Theoretical Chemistry', Structure of atoms (1st semester) and molecules (2nd semester), Université de Rennes 1 (2020-2023)
- Second year MSc (Master 2) course and hands-on sessions on 'Density functional theory based calculations for solids', RFCT-Winter school, Université de Rennes 1 (2020-2022)
- Course on the 'Computational Modelling Methods' and 'Theory of Perovskites', at the Centre for Doctoral Training in New and Sustainable Photovoltaics, Advanced Sustainable Materials, Department of Physics, University of Oxford (2019)
- First year MSc course on the 'Models and theory of molecular and atomic processes' at the Department of Physics, MSc 'Nanosciences & Nanotechnologies', Aristotle University of Thessaloniki, (2013-2014, 2017-2023)
- Lecture on the 'First Principles Calculations: Applications on Organic Electronic Materials' at the International Summer School on Nanosciences & Nanotechnologies: Organic electronics, ISSON-12 (2012)

Experience as a Team Leader

- Supervision of the doctoral thesis PhD of Mr. Bruno Cucco, Institut des Sciences Chimiques de Rennes, Université de Rennes 1 (2020-2023)
- Advisor doctoral thesis (DPhil) of Mr. Kevin Hurlbutt, Department of Materials, University of Oxford (2018-2021)
- Supervision of the undergrad thesis of Mr. Gabriel Joalland, Institut des Sciences Chimiques de Rennes, Université de Rennes 1 (2022)
- Supervision of the Master thesis of Mrs. Gaëlle Bouder, Institut des Sciences Chimiques de Rennes, Université de Rennes 1 (2021)
- Supervision of the Master's project of Mr Rocco Meli, Theoretical and Computational Chemistry (Doctoral Training Center), University of Oxford. (2017-2018)
- Sub-task leader for opto-electronic modelling of Work-Package 'Energy Generation', at the H2020 Core-1 & Core-2 Graphene Flagship project (grant agreements n^{O} 604391, 696656; 2016-2020)
- College advisor for four DPhil students within the Mathematical, Physical and Life Science division in Oxford, Wolfson College, University of Oxford (2016-2020).
- Coordinator for PRACE tier-0 computational project and tier-1 projects within the Prace-12, DECI-13, 14 and 16 calls. University of Oxford, Université de Rennes 1. Total resources managed: 13M core-hours (2015–2021)
- Coordinator for an Archer Leadership Computational Resources Project of 17M core-hours, Department of Materials, University of Oxford (2015–2017).

- Advisor on the Master's thesis project and doctoral thesis of Ms. Alexandra Stamateri, Aristotle University of Thessaloniki. (2014-2021)

National and European Projects

Coordination

2023-2026: ANR Project: "SURFIN: Surfaces and interfaces of novel perovskites and perovskitoids". Total budget: 187.162€.
2023-2026: ARED Project (Region): "ELTON: ELectronic sTructure Of Novel photo-active materials for sustainable energy". Total budget: 55.000€.
2022-2026: CPJ Project (ANR): "Conception in silico de matériaux pour la production d'énergie". Total budget: 200.000€.
2020-2022: Chaire de recherche Rennes Métropole. Project - AMDEA, Université de Rennes 1, ENSCR, INSA Rennes, ISCR, Total budget: 432.000€.
2011-2013: Operational Program "Education and Lifelong Learning" of the National Strategic Reference Framework (NSRF) - Research Funding Program: Heraclitus II. 45.000€ for PhD dissertation. European Social Fund (3/136/5).

Participation

2020-2023: Research scientist at the H2020 Innovation Action: Perocube (grant agreement n^{O} 861985)
2019-2020: Research scientist at the H2020 FET Open: DROP-IT (grant agreement n^{O} 862656)
2014-2020: Post-Doctoral research scientist and sub-task leader for opto-electronic modelling at the H2020 Core-2 Graphene Flagship project (grant agreements n^{O} 604391, 696656, 785219)
2013-2014: Doctoral research scientist at the FP7 NMP project SMARTONICS (grant agreements n^{O} 310229)

Computational Resources

2016-2021: Granted 4.000.000 CPU-hours PRACE DECI-16 call, UK HPC Archer2 (PI: G. Volonakis), Granted 20.000.000 CPU-hours PRACE-15, MareNostrum BSC. (Project: 2016163912, PI: F. Giustino, co-PI: G. Volonakis, S. Poncé, M. Schlipf) Granted 3.500.000 CPU-hours PRACE DECI-14 call, National Dutch HPC Cartesius. (PI: F. Giustino, co-PI: G. Volonakis) Granted 4.000.000 CPU-hours PRACE DECI-13 call, National Dutch HPC Cartesius. (PI: F. Giustino, co-PI: G. Volonakis)
2015: Granted 17.000.000 CPU-hours equivalent to 200.000€ on UK's national HPC Archer. Project: Advanced Materials for Solar Energy Conversion (PI: F. Giustino, Co-PIs: G. Volonakis, F. Caruso)

Organisational skills

- Guest-editor, with Ivan Mora-Sero and F. Giustino for JPhys Energy: focus collection Grand Challenges in Halide Perovskites: Lead-free (2021)
- Chairman (2019-2021) and member of the annual Workshop on Computational Modeling organization committee within the International Symposium on Organic Electronics, 2012-2021.
- Member of the organizing committee of the Annual International Conference Nanotexnology, 2006-2013.
- Member of the Scientific Committee of the summer school dedicated to Halide Perovskites, June 28th-July 4th 2020, Rennes, France.

International Collaborations

Over the last years, I have set up a large network of collaborators that covers experts from material synthesis to the device fabrication, but also developers of 'ab inito' codes. In the following I am listing some of the most important collaborators that could be related to the results of my future research projects:

Prof. H. J. Snaith (University of Oxford), **Prof. Th. Anthopoulos** (KAUST), **Prof. F. Giustino** (UT Austin), **Prof. A. di Carlo** (Tor Vergata University of Rome), **Prof. S. Logothetidis** (Aristotle University of Thessaloniki), **Prof. L. Tsetseris** (National Technical University of Athens), **Prof. N. Kalfagiannis** (Nottigham Trent University), **Prof. A. A. Haghighirad** (Karlsruhe Institute of Technology), **Prof. M. Pasta** (University of Oxford), **Prof. L. Herz** (University of Oxford), **Dr. S. Ponce** (EPFL/UCL, Belgium), **Dr. M. Zacharias** (INSA Rennes)

I have also been greatly successful in acquiring and managing computational resources through European and UK agencies. Since my PhD in 2014, I have been the principal investigator (PI), or co-PI in three PRACE/DECI tier-1 projects, one PRACE tier-0 project, 2 Archer RAP calls and 1 Archer Leadership project, totalling more than 50.000.000 CPU-hours.

Awards & Fellowships

- Laureate of the 'Chaire de Recherche' of Rennes Metropole, ISCR, ENCR, INSA, Université de Rennes 1 (2020-2023)
- Junior research fellowship (JRF) at Wolfson College, University of Oxford (2016-2020)
- Recognition award for excellence for the performance during calendar year. Department of Materials, University of Oxford (2017)
- "Young researcher award for best presentation" during the 3rd International Symposium for Flexible Organic Electronics, ISFOE, (2010)
- Scholarship for the first year of study MSc Nanosciences and Nanotechnologies (2010)

Research Track Record

Publications:	41	**Patents (granted):**	2 (2)
Book chapters:	2	**Invited communications (total):**	18 (27)
h-index:	17	**Citations (as of 01/02/2023):**	$>$3000

Journal Covers: 6 (ACS Energy Lett., Solar RRL, Adv. Mater. Interfaces, J. Phys. Chem. Lett., J. Phys. Cond. Matter.)

Oral communications at International Conferences

Keynote presentations

- Designing lead-free perovskites from first-principles. International Symposium for Flexible Organic Electronics – IS-FOE, 2017

Invited presentations

- Photovoltaic and excitonic properties of novel perovskite-like materials. European Materials Research Society Spring Meeting – EMRS, Strasbourg, 2023.
- Opto-electronic properties of novel perovskite(-like) materials for photovoltaics. International Symposium for Flexible Organic Electronics – IS-FOE 2023
- Materials design and ab initio modelling of novel perovskites and perovskitoids. KAUST Research Conference: Sustainable Energy Materials and Technologies for a Low Carbon Future - KAUST, SA 2023
- Excitonic properties of vacancy ordered double perovskites: electron-hole coupling and GW quasi-particles Materials for Sustainable Development Conference – MAT-SUS, Valencia, Spain 2023
- Electronic structure of bulk and layered perovskites. Materials Research Society Fall Meeting – MRS, Boston, USA 2022
- Materials design of halide double perovskites: Possible novel visible-light photo-catalysts. 3rd International Workshop Advances on Photocatalysis including Environmental and Energy Applications AdvPhotoCat-EE 2021
- Design rules for vacancy-ordered double perovskites International Symposium for Flexible Organic Electronics – IS-FOE 2021
- Computational design of novel semiconducting perovskites and their fundamental electronic properties. Journées Nationales du Photovoltaïque 2020 – JNPV, Dourdan, France 2021
- Computational design of semiconducting perovskites from first-principles. Moscow Autumn Perovskite Photovoltaics International Conference, Moscow, Russia, (visio) MAPPIC 2020
- Halide-oxide perovskite analogs nanoGe Fall Meeting, Barcelona, Spain (visio) – Nanoge 2020
- Computational design of novel semiconducting perovskites, fundamental electronic properties, and interfaces with 2D-materials, Materials Department, University of Crete, Greece, (visio) 2020
- Computational design of novel double perovskites European Materials Research Society Spring Meeting – E-MRS 2019
- A novel oxide double perovskite International Symposium for Flexible Organic Electronics – IS-FOE 2019
- Meeting on Electronic and Structural Dynamics in Hybrid Perovskites: Theory Meets Experiment – Telluride, Colorado, US, 2018
- Energy level alignment and surface properties of Pb-free halide double perovskites. International Symposium for Flexible Organic Electronics – IS-FOE, 2018
- Mixed halide & lead-free double perovskites from first-principles. International Symposium for Flexible Organic Electronics – IS-FOE, 2016
- Graphene/Perovskite Interfaces. International Symposium for Flexible Organic Electronics – IS-FOE, 2015

Contributed oral presentations

- European Materials Research Society Spring Meeting – EMRS, (virtual), 2021 Ruddorffites for solar-cell applications: Insights on their structures, electronic and optical properties from first-principles.
- Materials Research Society Fall Meeting – MRS, (virtual), 2020 Computational Design Rules for Novel Double Perovskites for Opto-Electronic Devices The Analogy Between Cs2AgInCl6 and Ba2AgIO6.
- Materials Research Society Fall Meeting – MRS, Boston, US, 2019 Computational design of perovskites: The case of Ba2AgIO6, a low band-gap solution processable oxide perovskite.
- American Physical Society March Meeting, Boston, US, 2019 Pb-free halide double perovskites: Computational materials design & surface properties.
- Materials Research Society Fall Meeting – MRS, Boston, US, 2017 In-based Lead-Free Halide Double Perovskites.
- European Materials Research Society Spring Meeting – E-MRS 2014 Impurity related degradation of P3HT and PCBM. A first principles study.
- International Symposium for Flexible Organic Electronics – IS-FOE, 2013 Continuous transformations of C60 crystals.
- International Symposium for Flexible Organic Electronics – IS-FOE, 2012 Oxygen and water impurities in P3HT & PCBM.
- International Symposium for Flexible Organic Electronics – IS-FOE, 2011 First principles calculations on optical properties of prototype organic semiconductors.

Detailed list of publications

1. Anharmonic electron-phonon coupling in ultrasoft and locally disordered perovskites, M Zacharias, G Volonakis, F Giustino, J Even, npj Computational Materials 9, 153 (2023) IF = 9.04
2. Surface and Optical Properties of Phase-Pure Silver Iodobismuthate Nanocrystals, A Matuhina, GK Grandhi, A Bergonzoni, L Pedesseau, R Grisorio, S Annurakshita, H Ali-Löytty, R Varghese, K Lahtonen, G Volonakis, V Pecunia, G Bautista, J Even, P Vivo, Nanoscale (Just Accepted 2023) IF = 8.3
3. Chemical Behavior and Local Structure of the Ruddlesden–Popper and Dion–Jacobson Alloyed Pb/Sn Bromide 2D Perovskites, P Fu, MA Quintero, ES Vasileiadou, P Raval, C Welton, M Kepenekian, G Volonakis, J Even, Y Liu, C Malliakas, Y Yang, C Laing, VP Dravid, GNM Reddy, C Li, EH Sargent, MG Kanatzidis, Journal of the American Chemical Society 145, 29, 15997–16014 (2023) IF = 16.4
4. Novel 3D Cubic Topology in Hybrid Lead Halides with a Symmetric Aromatic Triammonium Exhibiting Water Stability, ES Vasileiadou, IS Tajuddin, MC De Siena, VV Klepov, M Kepenekian, G Volonakis, J Even, L Wojtas, I Spanopoulos, X Zhou, AK Iyer, JL Fenton, WR Dichtel, MG Kanatzidis, Chemistry of Materials 35 (14), 5267–5280 (2023) IF = 9.81

5. Anharmonic lattice dynamics via the special displacement method, M Zacharias, G Volonakis, F Giustino, J Even, Physical Review B 108 (3), 035155 (2023) IF = 3.7

6. Fine Structure of Excitons in Vacancy-Ordered Halide Double Perovskites, B Cucco, C Katan, J Even, M Kepenekian*, G Volonakis*, ACS Materials Letters 5 (1), 52-59 (2023) IF = 11.17

7. Silver–Bismuth Halide Double Salts for Lead-Free Photovoltaics: Insights from Symmetry-Based Modeling, B Cucco, L Pedesseau, C Katan, J Even, M Kepenekian*, G Volonakis*, Solar RRL, 2200718 (2022) IF = 9.17

8. Short Aromatic Diammonium Ions Modulate Distortions in 2D Lead Bromide Perovskites for Tunable White-Light Emission, P Fu, MA Quintero, C Welton, X Li, B Cucco, MC De Siena, J Even, M. Kanatzidis, Chemistry of Materials 34 (21), 9685-9698 (2022) IF = 9.81

9. Ordered Mixed-Spacer 2D Bromide Perovskites and the Dual Role of 1, 2, 4-Triazolium Cation, X Li, H Dong, G Volonakis, CC Stoumpos, J Even, C Katan, P Guo, M. Kanatzidis, Chemistry of Materials 34 (14), 654 (2022) IF = 9.81

10. Pb-free halide perovskites for solar cells, light-emitting diodes, and photocatalysts, P Jiang, D Acharya, G Volonakis, M Zacharias, M Kepenekian, C. Katan, J. Even, APL Materials 10 (6), 060902 (2022) IF = 6.64

11. Origin of the high specific capacity in sodium manganese hexacyanomanganate, K Hurlbutt, F Giustino, G Volonakis*, M Pasta*, Chemistry of Materials 34 (10), 4336-4343 (2022) IF = 9.81

12. Electronic Structure and Stability of Cs_2TiX_6 and Cs_2ZrX_6 (X = Br,I) Vacancy Ordered Double Perovskites; B. Cucco, G. Bouder, L. Pedesseau, C. Katan, J. Even, M. Kepenekian, G. Volonakis*, Applied Physics Letters, 119 181903 (2021) IF = 3.79

13. Electronic structure and electron-transport properties of three metal hexacyanoferrates; K. Hurlbutt, F. Giustino, M. Pasta, G. Volonakis*, Chemistry of Materials, 33 7067 (2021) IF = 9.81

14. Phonon-limited Mobility and Electron-phonon Coupling in Lead-free Halide Double Perovskites; J. Leveille, G. Volonakis, F. Giustino; Journal Physical Chemistry Letters, 12 4474 (2021), Journal cover article IF = 6.48

15. Quasiparticle Band Structure and Phonon-Induced Band Gap Renormalization of the Lead-Free Halide Double Perovskite Cs2InAgCl6; VA Ha, G. Volonakis, H Lee, M Zacharias, F Giustino; The Journal of Physical Chemistry C, 125, 21689 (2021) IF = 4.2

16. Crystallographic, optical and electronic properties of the Cs2AgBi1-xInxBr6 double perovskite: understanding the fundamental photovoltaic efficiency challenges; L. Schade, S. Mahesh, G. Volonakis, M. Zacharias, B. Wenger, F. Schmidt, S. V. Kesala, D. Prabhakaran, M. A. Jalebi, M. Lenz, F. Giustino, G. Longo, P. G. Radaeli and H. J. Snaith; ACS Energy Letters, 6 1073 (2021) IF = 23.1

17. Ruddlesden–Popper Phase Hybrid Halide Perovskite/Small-Molecule Organic Blend Memory Transistor; M. Gedda, E. Yengel, H. Faber, F. Paulus, J. A. Kreß, M.-C. Tang, S. Zhang, C. A. Hacker, P. Kumar, D. R. Naphade, Y. Vaynzof, G. Volonakis, F. Giustino, T. D. Anthopoulos; Advanced Materials 2003137 (2020) IF = 30.9

18. Intrinsic quantum confinement in formamidinium lead triiodide perovskite; AD Wright, G Volonakis, J Borchert, CL Davies, F Giustino, MB Johnston, L. Herz; Nature Materials 19 (11), 1201-1206 (2020) IF = 43.8

19. Slot-die printed two-dimensional ZrS3 charge transport layer for perovskite light-emitting diodes; D. S. Muratov et al., A. R. Ishteev, D. A. Lypenko, V. O. Vanyushin, P. Gostishev, S. Perova, D. S. Saranin, D. Rossi, M. Auf der Maur, G. Volonakis, F. Giustino et al.,; ACS Applied Materials & Interfaces, 11, 48021 (2019) IF = 9.2

20. Oxide Analogs of Halide Perovskites and the New Semiconductor Ba2AgIO6 ; G. Volonakis, N.Sakai, H. J. Snaith, and F. Giustino ; Journal Physical Chemistry Letters, 10 1722 (2019), Journal cover article IF = 6.48

21. Interfaces between graphene-related materials and MAPbI3: Insights from first principles ; G. Volonakis and F. Giustino ; Advanced Materials and Interfaces 1800496 (2018), Cover of the section IF = 6.1

22. Graphene Oxide/Perovskite Interfaces for Photovoltaics ; N. Zibouche, G. Volonakis and F. Giustino ; The Journal of Physical Chemistry C 122 16715 (2018) IF = 4.2

23. Surface properties of lead-free halide double perovskites: Possible visible-light photo-catalysts for water splitting ; G. Volonakis and F. Giustino ; Applied Physics Letters 112 243901 (2018), Featured article IF = 3.79

24. High-Efficiency Fullerene Solar Cells Enabled by a Spontaneously Formed Mesostructured CuSCN-Nanowire Heterointerface ; W-Y. Sit, F.D. Eisner, Y-H. Lin, Y. Firdaus, A. Seitkhan, A.H. Balawi, F. Laquai, C.H. Burgess, M.A. McLachlan, G. Volonakis, F. Giustino, T.D. Anthopoulos ; Advanced Science 1700980 (2018) IF = 15.8

25. Route to Stable Lead-Free Double Perovskites with the Electronic Structure of CH3NH3PbI3: A Case for Mixed-Cation [Cs/CH3NH3/ CH(NH2)2]2InBiBr6 ; G. Volonakis, A. A. Haghighirad, H. J. Snaith, and F. Giustino ; Journal Physical Chemistry Letters, 8 3917 (2017) IF = 6.48

26. Cs2InAgCl6: A New Lead-Free Halide Double Perovskite with Direct Band Gap ; G. Volonakis, A. A. Haghighirad, R. L. Milot, W. H. Sio, M. R. Filip, B. Wenger, M. B. Johnston, L. M. Herz, H. J. Snaith, and F. Giustino ; Journal Physical Chemistry Letters 8 772 (2017) IF = 6.48

27. Perovskite-perovskite tandem photovoltaics with optimized bandgaps ; G. Eperon, T. Leijtens, K. A. Bush, R. Prasanna, T. Green, J. T.-W. Wang, D. P. McMeekin, G. Volonakis et al., (theory part: G. Volonakis and F. Giustino) ; Science, 354, 861 (2016) IF = 41.8

28. Lead-Free Halide Double Perovskites via Heterovalent Substitution of Noble Metals ; G. Volonakis, M. R.Filip, A. A. Haghighirad, N. Sakai, B. Wenger, H. J. Snaith, and F. Giustino ; Journal Physical Chemistry Letters 7 1254 (2016) IF = 6.48

29. Ferroelectric Graphene–Perovskite Interfaces. ; G. Volonakis and F. Giustino ; Journal Physical Chemistry Letters 6 2496 (2015) IF = 6.48

30. Graphene-based technologies for energy applications, challenges and perspectives. ; E. Quesnel, F. Roux, F. Emieux, P. Faucherand, E. Kymakis, G. Volonakis, F. Giustino, et al. ; 2D Materials 2 030204 (2015) IF = 7.1

31. Oxygen and water-related degradation of Poly(3-hexylthiophene) crystal. A first-principle study. ; G. Volonakis, L. Tsetseris, S. Logothetidis ; Physical Chemistry Chemical Physics 16 25557 (2014) IF = 3.6

32. Continuous transformations of C60 crystals: polymorphs, polymers, and ideal strength of fullerites. ; G. Volonakis, L. Tsetseris, S. Logothetidis ; Journal of Physics: Condensed Matter 25 435303 (2013) Journal cover article IF = 2.3

33. Impurity-related degradation in a prototype organic photovoltaic material: A first-principles study. ;G. Volonakis, L. Tsetseris, S. Logothetidis ; Organic Electronics 14 1242 (2013) IF = 3.7

34. Continuous transformation paths for the molecular crystal of the PCBM fullerene derivative. ; G. Volonakis, L. Tsetseris, S. Logothetidis ; Synthetic Metals 162 (24) 2421 (2012) IF = 2.5

35. Natural torsion in chiral single-wall carbon nanotubes ; N. Lazić, T. Vuković, G. Volonakis, I. Milošević, S. Logothetidis, and M. Damnjanović ; Journal of Physics: Condensed Matter 24 (48) 485302 (2012) IF = 2.3

36. Excess of boron in TiB2 superhard thin films: a combined experimental and ab initio study ; N. Kalfagiannis, G. Volonakis, L. Tsetseris, S. Logothetidis ; Journal of Physics D - Applied Physics 44 (38) 385402 (2011) IF = 3.2

37. Impurity-related vibrational modes in a pentacene crystal. ;G. Volonakis, L. Tsetseris, S. Logothetidis ; European Physical Journal-Applied Physics 55 (2) 23903 (2011) IF = 0.8

38. Electronic and structural properties of TiB2: Bulk, surface, and nanoscale effects. ;G. Volonakis, L. Tsetseris, S. Logothetidis ; Materials Science and Engineering B - Advanced Functional Solid-State Materials 176 (6) 484 (2011) IF = 4.0

39. On the Pentaheptite Nanotubes. ; M. Damnjanović, Z. Popovic, G. Volonakis, S. Logothetidis, and I. Milošević ; Materials and Manufacturing Processes 24 (10) 1124 (2009) IF = 4.6

40. Electromechanical switch based on pentaheptite nanotubes. ; I. Milošević, Z. Popović, G. Volonakis, S. Logothetidis, and M. Damnjanović ; Physical Review B 76 (11) 115406 (2007) IF = 4.0

41. Pentaheptide alotropes of carbon nanotubes. ; M. Damnjanović, G. Volonakis, S. Logothetidis, Z. Popović, and I. Milošević ; Six International Conference of the Balkan Physical: AIP Conference Proceedings 899 53 (2007) IF = 0.4

Book Chapters

1. Hybrid Halide Perovskites: Fundamental Theory and Design. M. R. Filip, G. Volonakis, F. Giustino The Handbook of Materials Modeling. Applications: Current and Emerging Materials Springer Publishing p. 295-324 2020

2. Structural and Electronic Properties of Organic Electronics Materials by Density Functional Theory Based Calculations. G. Volonakis, S. Logothetidis Handbook of flexible organic electronics Woodhead Publishing, 2015