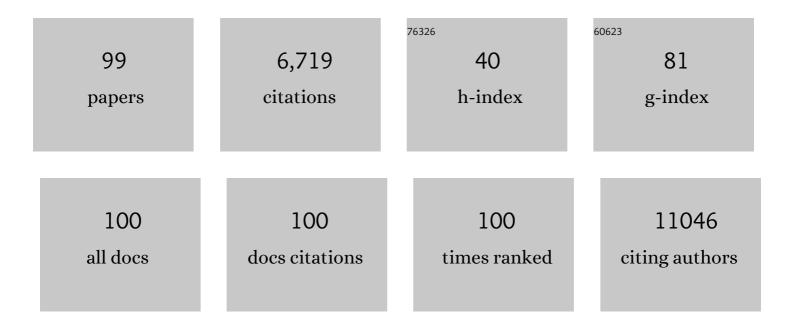
List of Publications by Year in descending order

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Μίνα Υρον

#	Article	IF	CITATIONS
1	Understanding Heterogeneities in Quantum Materials. Advanced Materials, 2023, 35, e2106909.	21.0	8
2	Selective Antisite Defect Formation in WS ₂ Monolayers via Reactive Growth on Dilute Wâ€Au Alloy Substrates. Advanced Materials, 2022, 34, e2106674.	21.0	14
3	Floquet band engineering and topological phase transitions in 1T' transition metal dichalcogenides. 2D Materials, 2022, 9, 025005.	4.4	4
4	Topography inversion in scanning tunneling microscopy of single-atom-thick materials from penetrating substrate states. Scientific Reports, 2022, 12, 7321.	3.3	2
5	Recent advances in computational materials design: methods, applications, algorithms, and informatics. Journal of Materials Science, 2022, 57, 10471-10474.	3.7	6
6	Stabilized Synthesis of 2D Verbeekite: Monoclinic PdSe ₂ Crystals with High Mobility and In-Plane Optical and Electrical Anisotropy. ACS Nano, 2022, 16, 13900-13910.	14.6	14
7	Doping transition-metal atoms in graphene for atomic-scale tailoring of electronic, magnetic, and quantum topological properties. Carbon, 2021, 173, 205-214.	10.3	35
8	Cobalt-based magnetic Weyl semimetals with high-thermodynamic stabilities. Npj Computational Materials, 2021, 7, .	8.7	13
9	Strain-Induced Growth of Twisted Bilayers during the Coalescence of Monolayer MoS ₂ Crystals. ACS Nano, 2021, 15, 4504-4517.	14.6	19
10	Understanding Substrate-Guided Assembly in van der Waals Epitaxy by <i>in Situ</i> Laser Crystallization within a Transmission Electron Microscope. ACS Nano, 2021, 15, 8638-8652.	14.6	7
11	GPU-acceleration of the ELPA2 distributed eigensolver for dense symmetric and hermitian eigenproblems. Computer Physics Communications, 2021, 262, 107808.	7.5	19
12	Revealing the Chemical Bonding in Adatom Arrays via Machine Learning of Hyperspectral Scanning Tunneling Spectroscopy Data. ACS Nano, 2021, 15, 11806-11816.	14.6	13
13	Self-regulated growth of candidate topological superconducting parkerite by molecular beam epitaxy. APL Materials, 2021, 9, 101110.	5.1	3
14	Antiferromagnetic Order and Linear Magnetoresistance in Fe-Substituted Shandite Co ₃ In ₂ S ₂ . Chemistry of Materials, 2021, 33, 9741-9749.	6.7	14
15	Crystal structures and rotational dynamics of a two-dimensional metal halide perovskite (OA)2PbI4. Journal of Chemical Physics, 2020, 152, 014703.	3.0	7
16	Solid-phase hetero epitaxial growth of α-phase formamidinium perovskite. Nature Communications, 2020, 11, 5514.	12.8	71
17	Quantum Phase Engineering of Two-Dimensional Post-Transition Metals by Substrates: Toward a Room-Temperature Quantum Anomalous Hall Insulator. Nano Letters, 2020, 20, 7186-7192.	9.1	9
18	Low Energy Implantation into Transition-Metal Dichalcogenide Monolayers to Form Janus Structures. ACS Nano, 2020, 14, 3896-3906.	14.6	136

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19	Emerging edge states on the surface of the epitaxial semimetal CuMnAs thin film. Applied Physics Letters, 2020, 116, 061603.	3.3	1
20	GPU acceleration of all-electron electronic structure theory using localized numeric atom-centered basis functions. Computer Physics Communications, 2020, 254, 107314.	7.5	30
21	Doping of Cr in Graphene Using Electron Beam Manipulation for Functional Defect Engineering. ACS Applied Nano Materials, 2020, 3, 10855-10863.	5.0	24
22	Temporally decoherent and spatially coherent vibrations in metal halide perovskites. Physical Review B, 2020, 102, .	3.2	7
23	Strain tolerance of two-dimensional crystal growth on curved surfaces. Science Advances, 2019, 5, eaav4028.	10.3	46
24	Performance of biologically inspired algorithms tuned on TiO2 nanoparticle benchmark system. Computational Materials Science, 2019, 165, 63-73.	3.0	2
25	Metastable Li _{1+δ} Mn ₂ O ₄ (0 â‰ቑ´ ≤) Spinel Phases Revealed by in Operando Neutron Diffraction and First-Principles Calculations. Chemistry of Materials, 2019, 31, 124-134.	6.7	28
26	Influence of defects and doping on phonon transport properties of monolayer MoSe ₂ . 2D Materials, 2018, 5, 031008.	4.4	30
27	Effect of Metal Doping and Vacancies on the Thermal Conductivity of Monolayer Molybdenum Diselenide. ACS Applied Materials & Interfaces, 2018, 10, 4921-4928.	8.0	29
28	First-Principles Prediction of New Electrides with Nontrivial Band Topology Based on One-Dimensional Building Blocks. Physical Review Letters, 2018, 120, 026401.	7.8	58
29	A hybrid optimization algorithm to explore atomic configurations of TiO2 nanoparticles. Computational Materials Science, 2018, 141, 1-9.	3.0	4
30	Laser Synthesis, Processing, and Spectroscopy of Atomically-Thin Two Dimensional Materials. Springer Series in Materials Science, 2018, , 1-37.	0.6	1
31	Phonon transport properties of two-dimensional electride Ca2N—A first-principles study. Applied Physics Letters, 2018, 113, .	3.3	11
32	Assessing the Predictive Power of Density Functional Theory in Finite-Temperature Hydrogen Adsorption/Desorption Thermodynamics. Journal of Physical Chemistry C, 2018, 122, 26189-26195.	3.1	5
33	Valence band inversion and spin-orbit effects in the electronic structure of monolayer GaSe. Physical Review B, 2018, 98, .	3.2	47
34	Strain-engineered optoelectronic properties of 2D transition metal dichalcogenide lateral heterostructures. 2D Materials, 2017, 4, 021016.	4.4	72
35	Understanding the Charge Transfer at the Interface of Electron Donors and Acceptors: TTF–TCNQ as an Example. ACS Applied Materials & Interfaces, 2017, 9, 27266-27272.	8.0	21
36	Surface Magnetism of Cobalt Nanoislands Controlled by Atomic Hydrogen. Nano Letters, 2017, 17, 292-298.	9.1	15

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37	A first-principles study of phonon transport properties of monolayer MoSe <inf>2</inf> . , 2017, , .		0
38	Nonequilibrium Synthesis of TiO ₂ Nanoparticle "Building Blocks―for Crystal Growth by Sequential Attachment in Pulsed Laser Deposition. Nano Letters, 2017, 17, 4624-4633.	9.1	33
39	Origin of long lifetime of band-edge charge carriers in organic–inorganic lead iodide perovskites. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 7519-7524.	7.1	137
40	Tunable quasiparticle band gap in few-layer GaSe/graphene van der Waals heterostructures. Physical Review B, 2017, 96, .	3.2	99
41	Interplay between intercalated oxygen superstructures and monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>h</mml:mi>-BN on Cu(100). Physical Review B, 2016, 94, .</mml:math 	3.2	16
42	Tailoring Vacancies Far Beyond Intrinsic Levels Changes the Carrier Type and Optical Response in Monolayer MoSe _{2â''<i>x</i>) crystals. Nano Letters, 2016, 16, 5213-5220.}	9.1	121
43	The Role of Interfacial Electronic Properties on Phonon Transport in Two-Dimensional MoS ₂ on Metal Substrates. ACS Applied Materials & Interfaces, 2016, 8, 33299-33306.	8.0	21
44	Entropy-driven structural transition and kinetic trapping in formamidinium lead iodide perovskite. Science Advances, 2016, 2, e1601650.	10.3	203
45	First-Principles Prediction of Thermodynamically Stable Two-Dimensional Electrides. Journal of the American Chemical Society, 2016, 138, 15336-15344.	13.7	91
46	Interlayer Coupling in Twisted WSe ₂ /WS ₂ Bilayer Heterostructures Revealed by Optical Spectroscopy. ACS Nano, 2016, 10, 6612-6622.	14.6	249
47	Phonon transport at the interfaces of vertically stacked graphene and hexagonal boron nitride heterostructures. Nanoscale, 2016, 8, 4037-4046.	5.6	38
48	Formation of Ideal Rashba States on Layered Semiconductor Surfaces Steered by Strain Engineering. Nano Letters, 2016, 16, 404-409.	9.1	44
49	Observation of two distinct negative trions in tungsten disulfide monolayers. Physical Review B, 2015, 92, .	3.2	44
50	Electronic Properties of Bilayer Graphene Strongly Coupled to Interlayer Stacking and an External Electric Field. Physical Review Letters, 2015, 115, 015502.	7.8	47
51	Growth of Metal Phthalocyanine on Deactivated Semiconducting Surfaces Steered by Selective Orbital Coupling. Physical Review Letters, 2015, 115, 096101.	7.8	30
52	Alloy Engineering of Defect Properties in Semiconductors: Suppression of Deep Levels in Transition-Metal Dichalcogenides. Physical Review Letters, 2015, 115, 126806.	7.8	81
53	Revealing the Preferred Interlayer Orientations and Stackings of Twoâ€Dimensional Bilayer Gallium Selenide Crystals. Angewandte Chemie, 2015, 127, 2750-2755.	2.0	5
54	Phase Transformations and Surface/Interface Properties in Functional Perovskites with Aberration-Corrected STEM/EELS. Microscopy and Microanalysis, 2015, 21, 2429-2430.	0.4	0

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55	Highly stable two-dimensional silicon phosphides: Different stoichiometries and exotic electronic properties. Physical Review B, 2015, 91, .	3.2	58
56	Revealing the Preferred Interlayer Orientations and Stackings of Twoâ€Dimensional Bilayer Gallium Selenide Crystals. Angewandte Chemie - International Edition, 2015, 54, 2712-2717.	13.8	45
57	Van der Waals Epitaxial Growth of Two-Dimensional Single-Crystalline GaSe Domains on Graphene. ACS Nano, 2015, 9, 8078-8088.	14.6	103
58	Patterned arrays of lateral heterojunctions within monolayer two-dimensional semiconductors. Nature Communications, 2015, 6, 7749.	12.8	213
59	Nitrogen Doping Enables Covalent-Like π–π Bonding between Graphenes. Nano Letters, 2015, 15, 5482-5491.	9.1	31
60	Structure and Formation Mechanism of Black TiO ₂ Nanoparticles. ACS Nano, 2015, 9, 10482-10488.	14.6	170
61	Exceptional Optoelectronic Properties of Hydrogenated Bilayer Silicene. Physical Review X, 2014, 4, .	8.9	35
62	Weak competing interactions control assembly of strongly bonded TCNQ ionic acceptor molecules on silver surfaces. Physical Review B, 2014, 90, .	3.2	11
63	Spatially resolved one-dimensional boundary states in graphene–hexagonal boron nitride planar heterostructures. Nature Communications, 2014, 5, 5403.	12.8	71
64	Binding and Diffusion of Lithium in Graphite: Quantum Monte Carlo Benchmarks and Validation of van der Waals Density Functional Methods. Journal of Chemical Theory and Computation, 2014, 10, 5318-5323.	5.3	117
65	Highly sensitive phototransistors based on two-dimensional GaTe nanosheets with direct bandgap. Nano Research, 2014, 7, 694-703.	10.4	140
66	Controlled Vapor Phase Growth of Single Crystalline, Two-Dimensional GaSe Crystals with High Photoresponse. Scientific Reports, 2014, 4, 5497.	3.3	222
67	Laser Interactions for the Synthesis and In Situ Diagnostics of Nanomaterials. Springer Series in Materials Science, 2014, , 143-173.	0.6	4
68	CO Oxidation on Supported Single Pt Atoms: Experimental and ab Initio Density Functional Studies of CO Interaction with Pt Atom on I,-Al ₂ 0 ₃ (010) Surface. Journal of the American Chemical Society, 2013, 135, 12634-12645.	13.7	535
69	Nature of the band gap and origin of the electro-/photo-activity of Co3O4. Journal of Materials Chemistry C, 2013, 1, 4628.	5.5	176
70	Surface-Induced Orientation Control of CuPc Molecules for the Epitaxial Growth of Highly Ordered Organic Crystals on Graphene. Journal of the American Chemical Society, 2013, 135, 3680-3687.	13.7	125
71	Highly Responsive Ultrathin GaS Nanosheet Photodetectors on Rigid and Flexible Substrates. Nano Letters, 2013, 13, 1649-1654.	9.1	683
72	How the shape of catalyst nanoparticles determines their crystallographic orientation during carbon nanofiber growth. Carbon, 2013, 60, 41-45.	10.3	7

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73	Hybrid density functional theory meets quasiparticle calculations: A consistent electronic structure approach. Physical Review B, 2013, 88, .	3.2	115
74	Finite-Temperature Hydrogen Adsorption and Desorption Thermodynamics Driven by Soft Vibration Modes. Physical Review Letters, 2013, 111, 066102.	7.8	25
75	Understanding the Metal-Directed Growth of Single-Crystal M-TCNQF ₄ Organic Nanowires with Time-Resolved, in Situ X-ray Diffraction and First-Principles Theoretical Studies. Journal of the American Chemical Society, 2012, 134, 14353-14361.	13.7	17
76	Benchmarking van der Waals density functionals with experimental data: potential-energy curves for H ₂ molecules on Cu(111), (100) and (110) surfaces. Journal of Physics Condensed Matter, 2012, 24, 424213.	1.8	35
77	Enhanced dipole moments in photo-excited TTF–TCNQ dimers. New Journal of Physics, 2011, 13, 073039.	2.9	8
78	First-principles studies of hydrogen interaction with ultrathin Mg and Mg-based alloy films. Physical Review B, 2011, 83, .	3.2	13
79	Equilibrium structure of ferrofluid aggregates. Journal of Physics Condensed Matter, 2010, 22, 455105.	1.8	12
80	Model for Self-Assembly of Carbon Nanotubes from Acetylene Based on Real-Time Studies of Vertically Aligned Growth Kinetics. Journal of Physical Chemistry C, 2009, 113, 15484-15491.	3.1	59
81	Interaction between hydrogen molecules and metallofullerenes. Journal of Chemical Physics, 2009, 131, 064707.	3.0	22
82	Calcium as the Superior Coating Metal in Functionalization of Carbon Fullerenes for High-Capacity Hydrogen Storage. Physical Review Letters, 2008, 100, 206806.	7.8	391
83	Energetics and kinetics of Ti clustering on neutral and charged C60 surfaces. Journal of Chemical Physics, 2008, 129, 134707.	3.0	34
84	Electron transfer and localization in endohedral metallofullerenes: <i>Ab initio</i> density functional theory calculations. Physical Review B, 2008, 78, .	3.2	23
85	Targeted medication delivery using magnetic nanostructures. Journal of Physics Condensed Matter, 2007, 19, 086210.	1.8	4
86	Polygonization and anomalous graphene interlayer spacing of multi-walled carbon nanofibers. Physical Review B, 2007, 75, .	3.2	26
87	Dynamics of Step Bunching in Heteroepitaxial Growth on Vicinal Substrates. Physical Review Letters, 2007, 99, 055503.	7.8	31
88	Charged Fullerenes as High-Capacity Hydrogen Storage Media. Nano Letters, 2007, 7, 2578-2583.	9.1	220
89	Energetics and packing of fullerenes in nanotube peapods. Physical Review B, 2005, 71, .	3.2	48
90	Persistent Step-Flow Growth of Strained Films on Vicinal Substrates. Physical Review Letters, 2005, 95, 095501.	7.8	119

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91	Zipper Mechanism of Nanotube Fusion: Theory and Experiment. Physical Review Letters, 2004, 92, 075504.	7.8	78
92	Microscopic mechanism of fullerene fusion. Physical Review B, 2004, 70, .	3.2	62
93	Diamond fragments as building blocks of functional nanostructures. Physical Review B, 2004, 70, .	3.2	137
94	Can photo excitations heal defects in carbon nanotubes?. Chemical Physics Letters, 2004, 392, 209-213.	2.6	23
95	Spectroscopic characterization of Stone-Wales defects in nanotubes. Physical Review B, 2004, 69, .	3.2	134
96	Magnetism in All-Carbon Nanostructures with Negative Gaussian Curvature. Physical Review Letters, 2003, 91, 237204.	7.8	200
97	Onset of nanotube decay under extreme thermal and electronic excitations. Physica B: Condensed Matter, 2002, 323, 78-85.	2.7	37
98	Boundary effects on dynamic behavior of Josephson-junction arrays. Physical Review B, 2000, 62, 5357-5360.	3.2	7
99	Lattice effects on the current-voltage characteristics of superconducting arrays. Physical Review B, 2000, 61, 3263-3266.	3.2	6