Leonidas Tsetseris

List of Publications by Year
in descending order

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141 papers	5,115 citations	81900 39 h-index	102487 66 g-index

142 all docs	142 docs citations	142 times ranked	6080 citing authors

#	Article	IF	Citations
1	Self-Assembled Monolayer Enables Hole Transport Layer-Free Organic Solar Cells with 18% Efficiency and Improved Operational Stability. ACS Energy Letters, 2020, 5, 2935-2944.	17.4	425
2	A Simple n-Dopant Derived from Diquat Boosts the Efficiency of Organic Solar Cells to 18.3%. ACS Energy Letters, 2020, 5, 3663-3671.	17.4	253
3	Copper(I) Thiocyanate (CuSCN) Holeâ€Transport Layers Processed from Aqueous Precursor Solutions and Their Application in Thinâ€Film Transistors and Highly Efficient Organic and Organometal Halide Perovskite Solar Cells. Advanced Functional Materials, 2017, 27, 1701818.	14.9	208
4	17.1% Efficient Singleâ€Junction Organic Solar Cells Enabled by nâ€Type Doping of the Bulkâ€Heterojunction. Advanced Science, 2020, 7, 1903419.	11.2	173
5	Graphene: An impermeable or selectively permeable membrane for atomic species?. Carbon, 2014, 67, 58-63.	10.3	162
6	Printable CsPbI₃ Perovskite Solar Cells with PCE of 19% via an Additive Strategy. Advanced Materials, 2020, 32, e2001243.	21.0	157
7	Doping Approaches for Organic Semiconductors. Chemical Reviews, 2022, 122, 4420-4492.	47.7	153
8	Remarkable Enhancement of the Hole Mobility in Several Organic Smallâ€Molecules, Polymers, and Smallâ€Molecule:Polymer Blend Transistors by Simple Admixing of the Lewis Acid pâ€Dopant B(C₆F₅)₃. Advanced Science, 2018, 5, 1700290.	11.2	131
9	18.4â€‰% Organic Solar Cells Using a High Ionization Energy Selfâ€Assembled Monolayer as Holeâ€Extraction Interlayer. ChemSusChem, 2021, 14, 3569-3578.	6.8	121
10	Physical mechanisms of negative-bias temperature instability. Applied Physics Letters, 2005, 86, 142103.	3.3	113
11	Lithiumâ€Ion Desolvation Induced by Nitrate Additives Reveals New Insights into High Performance Lithium Batteries. Advanced Functional Materials, 2021, 31, 2101593.	14.9	100
12	Water stable molecular n-doping produces organic electrochemical transistors with high transconductance and record stability. Nature Communications, 2020, 11, 3004.	12.8	82
13	Ligand-bridged charge extraction and enhanced quantum efficiency enable efficient nâ€“iâ€“p perovskite/silicon tandem solar cells. Energy and Environmental Science, 2021, 14, 4377-4390.	30.8	79
14	Structure and interaction of point defects in transition-metal nitrides. Physical Review B, 2007, 76, .	3.2	78
15	Adatom complexes and self-healing mechanisms on graphene and single-wall carbon nanotubes. Carbon, 2009, 47, 901-908.	10.3	78
16	Role of N Defects on Thermally Induced Atomic-Scale Structural Changes in Transition-Metal Nitrides. Physical Review Letters, 2007, 99, 125503.	7.8	73
17	Intercalation of oxygen and water molecules in pentacene crystals: First-principles calculations. Physical Review B, 2007, 75, .	3.2	66
18	Vacancies, interstitials and their complexes in titanium carbide. Acta Materialia, 2008, 56, 2864-2871.	7.9	66

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19	Common origin for enhanced low-dose-rate sensitivity and bias temperature instability under negative bias. IEEE Transactions on Nuclear Science, 2005, 52, 2265-2271.	2.0	65
20	Selective Nontemplated Adsorption of Organic Molecules on Nanofacets and the Role of Bonding Patterns. Physical Review Letters, 2006, 97, 156105.	7.8	65
21	Stability and electronic properties of ultrathin films of silicon and germanium. Physical Chemistry Chemical Physics, 2013, 15, 9710.	2.8	65
22	Addition of the Lewis Acid Zn(C₆F₅)₂ Enables Organic Transistors with a Maximum Hole Mobility in Excess of 20 cm² V^{â^'1} s^{â^'1}. Advanced Materials, 2019, 31, e1900871.	21.0	64
23	Defects and doping and their role in functionalizing graphene. MRS Bulletin, 2012, 37, 1187-1194.	3.5	61
24	Molecular dynamics simulations of stretched gold nanowires: The relative utility of different semiempirical potentials. Journal of Chemical Physics, 2007, 126, 144707.	3.0	57
25	Si/SiO₂ and SiC/SiO₂ Interfaces for MOSFETs â€“ Challenges and Advances. Materials Science Forum, 2006, 527-529, 935-948.	0.3	54
26	Hydrogen in MOSFETs â€“ A primary agent of reliability issues. Microelectronics Reliability, 2007, 47, 903-911.	1.7	54
27	Substitutional doping of graphene: The role of carbon divacancies. Physical Review B, 2014, 89, .	3.2	52
28	Enhancing the Charge Extraction and Stability of Perovskite Solar Cells Using Strontium Titanate (SrTiO₃) Electron Transport Layer. ACS Applied Energy Materials, 2019, 2, 8090-8097.	5.1	51
29	pâ€Doping of Copper(I) Thiocyanate (CuSCN) Holeâ€Transport Layers for Highâ€Performance Transistors and Organic Solar Cells. Advanced Functional Materials, 2018, 28, 1802055.	14.9	50
30	Hybrid organicâ€“metal oxide multilayer channel transistors with high operational stability. Nature Electronics, 2019, 2, 587-595.	26.0	49
31	Migration, incorporation, and passivation reactions of molecular hydrogen at theSiâ€SiO2interface. Physical Review B, 2004, 70, .	3.2	48
32	Negative bias-temperature instabilities in metalâ€“oxideâ€“silicon devices with SiO2 and SiOxNy/HfO2 gate dielectrics. Applied Physics Letters, 2004, 84, 4394-4396.	3.3	46
33	Oxygen Migration, Agglomeration, and Trapping: Key Factors for the Morphology of theSiâ^'SiO2Interface. Physical Review Letters, 2006, 97, 116101.	7.8	42
34	Defect Perovskites under Pressure: Structural Evolution of Cs₂SnX₆ (X = Cl,) Tj ETQq0 0 0 rgBT /Overlock 10 T	3.1	42
35	Stability and dynamics of carbon and nitrogen dopants in anataseTiO2: A density functional theory study. Physical Review B, 2010, 81, .	3.2	41
36	Use of the Phenâ€NaDPO:Sn(SCN)₂ Blend as Electron Transport Layer Results to Consistent Efficiency Improvements in Organic and Hybrid Perovskite Solar Cells. Advanced Functional Materials, 2019, 29, 1905810.	14.9	41

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37	Hydrogen-Related Instabilities in MOS Devices Under Bias Temperature Stress. IEEE Transactions on Device and Materials Reliability, 2007, 7, 502-508.	2.0	40
38	A universal solution processed interfacial bilayer enabling ohmic contact in organic and hybrid optoelectronic devices. Energy and Environmental Science, 2020, 13, 268-276.	30.8	40
39	Effects of Switched-bias Annealing on Charge Trapping in HfO$_{2}$ Gate Dielectrics. IEEE Transactions on Nuclear Science, 2006, 53, 3636-3643.	2.0	39
40	Excess of boron in TiB₂ superhard thin films: a combined experimental and ab initio study. Journal Physics D: Applied Physics, 2011, 44, 385402.	2.8	39
41	Introduction of nitrogen with controllable configuration into graphene via vacancies and edges. Journal of Materials Chemistry A, 2013, 1, 14927.	10.3	39
42	Effects of device aging on microelectronics radiation response and reliability. Microelectronics Reliability, 2007, 47, 1075-1085.	1.7	38
43	Reactions of Water Molecules in Silica-Based Network Glasses. Physical Review Letters, 2008, 100, 105503.	7.8	38
44	Morphology and defect properties of the Geâ€“GeO2 interface. Applied Physics Letters, 2009, 95, .	3.3	38
45	Configuration and conductance evolution of benzene-dithiol molecular junctions under elongation. Physical Review B, 2010, 82, .	3.2	38
46	Structural evolution of single-layer films during deposition of silicon on silver: a first-principles study. Journal of Physics Condensed Matter, 2012, 24, 442001.	1.8	38
47	Reliability and radiation effects in IC technologies. , 2008, , .		37
48	Large impurity effects in rubrene crystals: First-principles calculations. Physical Review B, 2008, 78, .	3.2	37
49	Thermal donor formation processes in silicon and the catalytic role of hydrogen. Applied Physics Letters, 2006, 88, 051916.	3.3	35
50	Introducing a Nonvolatile Nâ€Type Dopant Drastically Improves Electron Transport in Polymer and Smallâ€Molecule Organic Transistors. Advanced Functional Materials, 2019, 29, 1902784.	14.9	35
51	Using Two Compatible Donor Polymers Boosts the Efficiency of Ternary Organic Solar Cells to 17.7%. Chemistry of Materials, 2021, 33, 7254-7262.	6.7	35
52	Hydrogen effects in MOS devices. Microelectronic Engineering, 2007, 84, 2344-2349.	2.4	34
53	Adsorbate-Induced Defect Formation and Annihilation on Graphene and Single-Walled Carbon Nanotubes. Journal of Physical Chemistry B, 2009, 113, 941-944.	2.6	34
54	Graphene nano-ribbon formation through hydrogen-induced unzipping of carbon nanotubes. Applied Physics Letters, 2011, 99, 143119.	3.3	34

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55	Molecular doping of graphene with ammonium groups. Physical Review B, 2012, 85, .	3.2	34
56	Migration of species in a prototype diffusion barrier: Cu, O, and H in TiN. Applied Physics Letters, 2009, 94, .	3.3	33
57	The Origin of Electron Mobility Enhancement in Strained MOSFETs. IEEE Electron Device Letters, 2007, 28, 1018-1020.	3.9	32
58	Encapsulation of Floating Carbon Nanotubes inSiO2. Physical Review Letters, 2006, 97, 266805.	7.8	30
59	Noncollinear magnetism of iron along the tetragonal Bain transformation. Physical Review B, 2005, 72, .	3.2	29
60	Interlayer exchange coupling in Fe/Cr multilayers. Physical Review B, 1997, 55, 11586-11592.	3.2	28
61	Response of silicane and germanane to uni-axial compression: Superstructures, polymorph nano-ribbons, and extreme bending. Journal of Chemical Physics, 2013, 139, 124709.	3.0	26
62	Copper thiocyanate: polytypes, defects, impurities, and surfaces. Journal of Physics Condensed Matter, 2016, 28, 295801.	1.8	26
63	Performance, reliability, radiation effects, and aging issues in microelectronics â€“ From atomic-scale physics to engineering-level modeling. Solid-State Electronics, 2010, 54, 841-848.	1.4	24
64	Oxygen and water-related impurities inC60crystals: A density-functional theory study. Physical Review B, 2010, 82, .	3.2	24
65	Silicene on metal substrates: A first-principles study on the emergence of a hierarchy of honeycomb structures. Applied Surface Science, 2014, 291, 93-97.	6.1	24
66	Atomic-scale mechanisms of selective adsorption and dimerization of pentacene on Si surfaces. Applied Physics Letters, 2005, 87, 233109.	3.3	23
67	Dual role of fluorine at the Siâ€“SiO2 interface. Applied Physics Letters, 2004, 85, 4950-4952.	3.3	22
68	Hydrogen uptake by graphene and nucleation of graphane. Journal of Materials Science, 2012, 47, 7571-7579.	3.7	22
69	Millisecond non-melt laser annealing of phosphorus implanted germanium: Influence of nitrogen co-doping. Journal of Applied Physics, 2015, 118, .	2.5	22
70	Phthalo-carbonitride: an ab initio prediction of a stable two-dimensional material. 2D Materials, 2016, 3, 021006.	4.4	22
71	Modification of the electronic properties of rubrene crystals by water and oxygen-related species. Organic Electronics, 2009, 10, 333-340.	2.6	21
72	Chemical routes to modify, uplift, and detach a silicene layer from a metal substrate. Physical Chemistry Chemical Physics, 2014, 16, 5183.	2.8	21

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73	Electronic and structural properties of TiB2: Bulk, surface, and nanoscale effects. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2011, 176, 484-489.	3.5	20
74	Two-dimensional copper thio- and seleno-cyanates. Physical Chemistry Chemical Physics, 2016, 18, 7837-7840.	2.8	20
75	Trapping and release of impurities in TiN: A first-principles study. Physical Review B, 2008, 78, .	3.2	19
76	Copper (I) Selenocyanate (CuSeCN) as a Novel Holeâ€Transport Layer for Transistors, Organic Solar Cells, and Lightâ€Emitting Diodes. Advanced Functional Materials, 2018, 28, 1707319.	14.9	19
77	A Multilayered Electron Extracting System for Efficient Perovskite Solar Cells. Advanced Functional Materials, 2020, 30, 2004273.	14.9	17
78	N-Doping improves charge transport and morphology in the organic non-fullerene acceptor O-IDTBR. Journal of Materials Chemistry C, 2021, 9, 4486-4495.	5.5	17
79	Design Considerations for CdTe Nanotetrapods as Electronic Devices. Nano Letters, 2009, 9, 3683-3688.	9.1	16
80	Intermolecular bridges and carrier traps in defective C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>60</mml:mn></mml:msub></mml:math>crystals. Physical Review B, 2011, 84, .	3.2	15
81	Configurations, electronic properties, and diffusion of carbon and nitrogen dopants in rutile TiO2: A density functional theory study. Physical Review B, 2011, 84, .	3.2	15
82	Magnetic two-dimensional C₃N₂ carbonitrides: semiconductors, metals and half-metals. Physical Chemistry Chemical Physics, 2017, 19, 26743-26748.	2.8	15
83	Highly sensitive and room temperature detection of ultra-low concentrations of O₃ using self-powered sensing elements of Cu₂O nanocubes. Nanoscale Advances, 2019, 1, 2009-2017.	4.6	15
84	Atomic-Scale Mechanisms for Low-NIEL Dopant-Type Dependent Damage in Si. IEEE Transactions on Nuclear Science, 2006, 53, 3621-3628.	2.0	14
85	Ge volatilization products in high-k gate dielectrics. Microelectronic Engineering, 2011, 88, 427-430.	2.4	14
86	Impurity-related effects in poly(3-hexylthiophene) crystals. Physical Chemistry Chemical Physics, 2014, 16, 25557-25563.	2.8	13
87	Analytical Greenâ€™s-function calculation of the interlayer exchange coupling in Fe/Cr multilayers. Physical Review B, 1997, 56, R11392-R11395.	3.2	12
88	Near-IR Absorbing Molecular Semiconductors Incorporating Cyanated Benzothiadiazole Acceptors for High-Performance Semitransparent n-Type Organic Field-Effect Transistors. , 2022, 4, 165-174.		12
89	First-principles studies of isomerization processes of silicon clusters. Physical Review B, 2007, 76, .	3.2	11
90	First-principles study of siloxene and germoxene: stable conformations, electronic properties, and defects. Journal of Physics Condensed Matter, 2014, 26, 285301.	1.8	11

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91	Two-dimensional cyanates: stabilization through hydrogenation. Physical Chemistry Chemical Physics, 2016, 18, 14662-14666.	2.8	11
92	Reactions of excess hydrogen at aSi(111)surface with H termination: First-principles calculations. Physical Review B, 2006, 74, .	3.2	10
93	Atomic-scale mechanisms for diffusion of impurities in transition-metal nitrides. Surface and Coatings Technology, 2010, 204, 2089-2094.	4.8	10
94	Impurity-related degradation in a prototype organic photovoltaic material: A first-principles study. Organic Electronics, 2013, 14, 1242-1248.	2.6	10
95	Hydrogenationâˆ•deuteration of the Siâ€“SiO2 interface: Atomic-scale mechanisms and limitations. Applied Physics Letters, 2005, 86, 112107.	3.3	9
96	Stability and Dynamics of Frenkel Pairs in Si. Physical Review Letters, 2007, 99, 215503.	7.8	9
97	Interaction of metal impurities with native oxygen defects in GeO2. Microelectronic Engineering, 2013, 104, 37-41.	2.4	9
98	Hydrogen- and oxygen-related effects in phthalocyanine crystals: formation of carrier traps and a change in the magnetic state. Physical Chemistry Chemical Physics, 2014, 16, 3317.	2.8	9
99	Functionalization of Nanographenes: Metallic and Insulating Hexabenzocoronene Derivatives. Journal of Physical Chemistry C, 2014, 118, 1347-1352.	3.1	9
100	Ca- and Sc-based ternary AlB2-like crystals: a first-principles study. Journal of Physics Condensed Matter, 2017, 29, 045701.	1.8	9
101	14ÂGHz Schottky Diodes Using a pâ€Doped Organic Polymer. Advanced Materials, 2022, 34, e2108524.	21.0	9
102	First-principles studies on organic electronic materials. EPJ Applied Physics, 2009, 46, 12511.	0.7	8
103	Functionalization of two-dimensional phthalo-carbonitride with metal atoms. Physical Chemistry Chemical Physics, 2016, 18, 26088-26093.	2.8	8
104	A Lowâ€Power CuSCN Hydrogen Sensor Operating Reversibly at Room Temperature. Advanced Functional Materials, 2022, 32, 2102635.	14.9	8
105	Chlorine-Infused Wide-Band Gap p-CuSCN/n-GaN Heterojunction Ultraviolet-Light Photodetectors. ACS Applied Materials & Interfaces, 2022, 14, 17889-17898.	8.0	8
106	Stability of Group-V Endohedral Fullerenes. Journal of Physical Chemistry C, 2011, 115, 3528-3533.	3.1	7
107	Defect formation and hysteretic inter-tube displacement in multi-wall carbon nanotubes. Carbon, 2011, 49, 581-586.	10.3	7
108	Computational Studies of Nanographene Systems: Extended Discotics, Covalently Linked â€œSupermolecules,â€• and Functionalized Supramolecular Assemblies. Journal of Physical Chemistry C, 2018, 122, 18715-18731.	3.1	7

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109	A direct transfer solution for digital laser printing of CVD graphene. 2D Materials, 2021, 8, 045017.	4.4	7
110	Defect formation and annihilation at interfaces. Microelectronic Engineering, 2011, 88, 395-398.	2.4	6
111	Continuous transformations of C₆₀crystals: polymorphs, polymers, and the ideal strength of fullerites. Journal of Physics Condensed Matter, 2013, 25, 435303.	1.8	6
112	Formation and properties of graphane superstructures. Journal of Physics Condensed Matter, 2013, 25, 085301.	1.8	6
113	Novel Au- and Ge-based two-dimensional materials formed through topotactic transitions of AlB₂-like structures. Nanoscale, 2016, 8, 13558-13561.	5.6	6
114	Stacks of graphene with silicane or germanane: a first-principles study. Journal of Physics Condensed Matter, 2016, 28, 035304.	1.8	6
115	Two-dimensional metal-phosphorus monohydrides. FlatChem, 2017, 2, 49-53.	5.6	6
116	Addition of Diquat Enhances the Electron Mobility in Various Nonâ€Fullerene Acceptor Molecules. Advanced Functional Materials, 0, , 2202954.	14.9	6
117	Ge-related impurities in high-k oxides: Carrier traps and interaction with native defects. Microelectronic Engineering, 2011, 88, 1432-1435.	2.4	5
118	Hydrogenâ€“dopant interactions in SiGe and strained Si. Applied Physics Letters, 2010, 96, .	3.3	4
119	Defect-related hysteresis in nanotube-based nano-electromechanical systems. Nanoscale Research Letters, 2011, 6, 245.	5.7	4
120	Continuous transformation paths for the molecular crystals of the PCBM fullerene derivative. Synthetic Metals, 2012, 162, 2421-2427.	3.9	4
121	Two-dimensional Mo(SCN)₂: a novel MoS₂-variant. Journal of Physics Condensed Matter, 2017, 29, 085702.	1.8	4
122	Field-induced reactions of water molecules at Si-dielectric interfaces. Materials Research Society Symposia Proceedings, 2003, 786, 331.	0.1	3
123	Probing the nano-scale with first-principles calculations. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2008, 152, 109-113.	3.5	3
124	Performance, reliability, radiation effects, and aging issues in microelectronics - from atomic-scale physics to engineering-level modeling. , 2009, , .		2
125	Performance, reliability, radiation effects, and aging issues in microelectronics — from atomic-scale physics to engineering-level modeling. , 2009, , .		2
126	DEFECT-RELATED ISSUES IN HIGH-K DIELECTRICS. , 2006, , 189-202.		1

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127	Effects of Device Aging on Microelectronics Radiation Response and Reliability. , 0, , .		1
128	Engineering model of a biased metalâ€“moleculeâ€“metal junction. Journal of Computational Electronics, 2007, 6, 425-430.	2.5	1
129	Performance, Reliability, Radiation Effects, and Aging Issues in Microelectronics - From Atomic-Scale Physics to Engineering-Level Modeling. ECS Transactions, 2009, 19, 319-337.	0.5	1
130	Impurity-related vibrational modes in a pentacene crystal. EPJ Applied Physics, 2011, 55, 23903.	0.7	1
131	Arrays of carbon nanoscrolls as deep subwavelength magnetic metamaterials. Physical Review B, 2013, 88, .	3.2	1
132	Low-energy consumption CuSCN-based ultra-low-ppb level ozone sensor, operating at room temperature. Sensors and Actuators A: Physical, 2022, 338, 113462.	4.1	1
133	RelativisticNthorder muffin-tin orbital theory. Physical Review B, 2005, 71, .	3.2	0
134	Physical Mechanisms Responsible for the Abruptness of the Si-SiO2 Interface. AIP Conference Proceedings, 2007, , .	0.4	0
135	(Invited) Defects and Impurities in Ge-Based Electronic Devices. ECS Transactions, 2011, 41, 47-52.	0.5	0
136	Atomic-Scale Mechanisms of Growth and Doping of Graphene Nano-Ribbons. ECS Transactions, 2011, 41, 71-75.	0.5	0
137	(Invited) Doping, Functionalization, and Permeability of Graphene: Insights from First-Principles Studies. ECS Transactions, 2014, 64, 121-125.	0.5	0
138	Two-dimensional thio- and seleno-cyanates of Mo and W. Journal of Physics Condensed Matter, 2017, 29, 485703.	1.8	0
139	Impact of Radiation-Induced Defects on Bipolar Device Operation. , 2008, , .		0
140	Defect Formation and Annihilation in Electronic Devices and the Role of Hydrogen. , 2008, , .		0
141	Formation and properties of iodine- and acetonitrile-functionalized two-dimensional Si materials: a Density Functional Theory study. Physical Chemistry Chemical Physics, 2021, 24, 411-418.	2.8	0