Leonidas Tsetseris

List of Publications by Year
in descending order

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Version: 2024-02-01

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	A Lowâ€Power CuSCN Hydrogen Sensor Operating Reversibly at Room Temperature. Advanced Functional Materials, 2022, 32, 2102635.	14.9	8
2	Doping Approaches for Organic Semiconductors. Chemical Reviews, 2022, 122, 4420-4492.	47.7	153
3	14ÂGHz Schottky Diodes Using a pâ€Doped Organic Polymer. Advanced Materials, 2022, 34, e2108524.	21.0	9
4	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
5	Near-IR Absorbing Molecular Semiconductors Incorporating Cyanated Benzothiadiazole Acceptors for High-Performance Semitransparent n-Type Organic Field-Effect Transistors. , 2022, 4, 165-174.		12
6	Chlorine-Infused Wide-Band Gap p-CuSCN/n-GaN Heterojunction Ultraviolet-Light Photodetectors. ACS Applied Materials & Interfaces, 2022, 14, 17889-17898.	8.0	8
7	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
8	Lithiumâ€Ion Desolvation Induced by Nitrate Additives Reveals New Insights into High Performance Lithium Batteries. Advanced Functional Materials, 2021, 31, 2101593.	14.9	100
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	A direct transfer solution for digital laser printing of CVD graphene. 2D Materials, 2021, 8, 045017.	4.4	7
11	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
12	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
13	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
14	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
15	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
16	A Multilayered Electron Extracting System for Efficient Perovskite Solar Cells. Advanced Functional Materials, 2020, 30, 2004273.	14.9	17
17	Printable CsPbI₃ Perovskite Solar Cells with PCE of 19% via an Additive Strategy. Advanced Materials, 2020, 32, e2001243.	21.0	157
18	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

#	Article	IF	Citations
19	Water stable molecular n-doping produces organic electrochemical transistors with high transconductance and record stability. Nature Communications, 2020, 11, 3004.	12.8	82
20	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
21	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
22	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
23	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
24	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
25	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
26	Hybrid organicâ€“metal oxide multilayer channel transistors with high operational stability. Nature Electronics, 2019, 2, 587-595.	26.0	49
27	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
28	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
29	Defect Perovskites under Pressure: Structural Evolution of Cs₂SnX₆ (X = Cl,) Tj ETQq1 1 0.784314 rgBT /Ov	3.1	42
30	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
31	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
32	Two-dimensional Mo(SCN)₂: a novel MoS₂-variant. Journal of Physics Condensed Matter, 2017, 29, 085702.	1.8	4
33	Two-dimensional metal-phosphorus monohydrides. FlatChem, 2017, 2, 49-53.	5.6	6
34	Ca- and Sc-based ternary AlB2-like crystals: a first-principles study. Journal of Physics Condensed Matter, 2017, 29, 045701.	1.8	9
35	Two-dimensional thio- and seleno-cyanates of Mo and W. Journal of Physics Condensed Matter, 2017, 29, 485703.	1.8	0
36	Magnetic two-dimensional C₃N₂ carbonitrides: semiconductors, metals and half-metals. Physical Chemistry Chemical Physics, 2017, 19, 26743-26748.	2.8	15

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37	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
38	Two-dimensional cyanates: stabilization through hydrogenation. Physical Chemistry Chemical Physics, 2016, 18, 14662-14666.	2.8	11
39	Phthalo-carbonitride: an ab initio prediction of a stable two-dimensional material. 2D Materials, 2016, 3, 021006.	4.4	22
40	Functionalization of two-dimensional phthalo-carbonitride with metal atoms. Physical Chemistry Chemical Physics, 2016, 18, 26088-26093.	2.8	8
41	Copper thiocyanate: polytypes, defects, impurities, and surfaces. Journal of Physics Condensed Matter, 2016, 28, 295801.	1.8	26
42	Novel Au- and Ge-based two-dimensional materials formed through topotactic transitions of AlB₂-like structures. Nanoscale, 2016, 8, 13558-13561.	5.6	6
43	Two-dimensional copper thio- and seleno-cyanates. Physical Chemistry Chemical Physics, 2016, 18, 7837-7840.	2.8	20
44	Stacks of graphene with silicane or germanane: a first-principles study. Journal of Physics Condensed Matter, 2016, 28, 035304.	1.8	6
45	Millisecond non-melt laser annealing of phosphorus implanted germanium: Influence of nitrogen co-doping. Journal of Applied Physics, 2015, 118, .	2.5	22
46	(Invited) Doping, Functionalization, and Permeability of Graphene: Insights from First-Principles Studies. ECS Transactions, 2014, 64, 121-125.	0.5	0
47	Chemical routes to modify, uplift, and detach a silicene layer from a metal substrate. Physical Chemistry Chemical Physics, 2014, 16, 5183.	2.8	21
48	Substitutional doping of graphene: The role of carbon divacancies. Physical Review B, 2014, 89, .	3.2	52
49	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
50	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
51	Impurity-related effects in poly(3-hexylthiophene) crystals. Physical Chemistry Chemical Physics, 2014, 16, 25557-25563.	2.8	13
52	Functionalization of Nanographenes: Metallic and Insulating Hexabenzocoronene Derivatives. Journal of Physical Chemistry C, 2014, 118, 1347-1352.	3.1	9
53	First-principles study of siloxene and germoxene: stable conformations, electronic properties, and defects. Journal of Physics Condensed Matter, 2014, 26, 285301.	1.8	11
54	Graphene: An impermeable or selectively permeable membrane for atomic species?. Carbon, 2014, 67, 58-63.	10.3	162

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55	Continuous transformations of C₆₀crystals: polymorphs, polymers, and the ideal strength of fullerites. Journal of Physics Condensed Matter, 2013, 25, 435303.	1.8	6
56	Introduction of nitrogen with controllable configuration into graphene via vacancies and edges. Journal of Materials Chemistry A, 2013, 1, 14927.	10.3	39
57	Interaction of metal impurities with native oxygen defects in GeO2. Microelectronic Engineering, 2013, 104, 37-41.	2.4	9
58	Formation and properties of graphane superstructures. Journal of Physics Condensed Matter, 2013, 25, 085301.	1.8	6
59	Impurity-related degradation in a prototype organic photovoltaic material: A first-principles study. Organic Electronics, 2013, 14, 1242-1248.	2.6	10
60	Stability and electronic properties of ultrathin films of silicon and germanium. Physical Chemistry Chemical Physics, 2013, 15, 9710.	2.8	65
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	Arrays of carbon nanoscrolls as deep subwavelength magnetic metamaterials. Physical Review B, 2013, 88, .	3.2	1
63	Defects and doping and their role in functionalizing graphene. MRS Bulletin, 2012, 37, 1187-1194.	3.5	61
64	Hydrogen uptake by graphene and nucleation of graphane. Journal of Materials Science, 2012, 47, 7571-7579.	3.7	22
65	Continuous transformation paths for the molecular crystals of the PCBM fullerene derivative. Synthetic Metals, 2012, 162, 2421-2427.	3.9	4
66	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
67	Molecular doping of graphene with ammonium groups. Physical Review B, 2012, 85, .	3.2	34
68	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
69	Stability of Group-V Endohedral Fullerenes. Journal of Physical Chemistry C, 2011, 115, 3528-3533.	3.1	7
70	Impurity-related vibrational modes in a pentacene crystal. EPJ Applied Physics, 2011, 55, 23903.	0.7	1
71	Graphene nano-ribbon formation through hydrogen-induced unzipping of carbon nanotubes. Applied Physics Letters, 2011, 99, 143119.	3.3	34
72	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

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73	Defect-related hysteresis in nanotube-based nano-electromechanical systems. Nanoscale Research Letters, 2011, 6, 245.	5.7	4
74	Defect formation and hysteretic inter-tube displacement in multi-wall carbon nanotubes. Carbon, 2011, 49, 581-586.	10.3	7
75	Defect formation and annihilation at interfaces. Microelectronic Engineering, 2011, 88, 395-398.	2.4	6
76	Ge-related impurities in high-k oxides: Carrier traps and interaction with native defects. Microelectronic Engineering, 2011, 88, 1432-1435.	2.4	5
77	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
78	Ge volatilization products in high-k gate dielectrics. Microelectronic Engineering, 2011, 88, 427-430.	2.4	14
79	(Invited) Defects and Impurities in Ge-Based Electronic Devices. ECS Transactions, 2011, 41, 47-52.	0.5	0
80	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
81	Atomic-Scale Mechanisms of Growth and Doping of Graphene Nano-Ribbons. ECS Transactions, 2011, 41, 71-75.	0.5	0
82	Atomic-scale mechanisms for diffusion of impurities in transition-metal nitrides. Surface and Coatings Technology, 2010, 204, 2089-2094.	4.8	10
83	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
84	Oxygen and water-related impurities inC60crystals: A density-functional theory study. Physical Review B, 2010, 82, .	3.2	24
85	Configuration and conductance evolution of benzene-dithiol molecular junctions under elongation. Physical Review B, 2010, 82, .	3.2	38
86	Stability and dynamics of carbon and nitrogen dopants in anataseTiO2: A density functional theory study. Physical Review B, 2010, 81, .	3.2	41
87	Hydrogenâ€“dopant interactions in SiGe and strained Si. Applied Physics Letters, 2010, 96, .	3.3	4
88	Migration of species in a prototype diffusion barrier: Cu, O, and H in TiN. Applied Physics Letters, 2009, 94, .	3.3	33
89	Morphology and defect properties of the Geâ€“GeO2 interface. Applied Physics Letters, 2009, 95, .	3.3	38
90	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

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91	Modification of the electronic properties of rubrene crystals by water and oxygen-related species. Organic Electronics, 2009, 10, 333-340.	2.6	21
92	Adatom complexes and self-healing mechanisms on graphene and single-wall carbon nanotubes. Carbon, 2009, 47, 901-908.	10.3	78
93	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
94	Performance, reliability, radiation effects, and aging issues in microelectronics - from atomic-scale physics to engineering-level modeling. , 2009, , .		2
95	Performance, reliability, radiation effects, and aging issues in microelectronics — from atomic-scale physics to engineering-level modeling. , 2009, , .		2
96	Design Considerations for CdTe Nanotetrapods as Electronic Devices. Nano Letters, 2009, 9, 3683-3688.	9.1	16
97	First-principles studies on organic electronic materials. EPJ Applied Physics, 2009, 46, 12511.	0.7	8
98	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
99	Vacancies, interstitials and their complexes in titanium carbide. Acta Materialia, 2008, 56, 2864-2871.	7.9	66
100	Trapping and release of impurities in TiN: A first-principles study. Physical Review B, 2008, 78, .	3.2	19
101	Reliability and radiation effects in IC technologies. , 2008, , .		37
102	Reactions of Water Molecules in Silica-Based Network Glasses. Physical Review Letters, 2008, 100, 105503.	7.8	38
103	Large impurity effects in rubrene crystals: First-principles calculations. Physical Review B, 2008, 78, .	3.2	37
104	Impact of Radiation-Induced Defects on Bipolar Device Operation. , 2008, , .		0
105	Defect Formation and Annihilation in Electronic Devices and the Role of Hydrogen. , 2008, , .		0
106	Stability and Dynamics of Frenkel Pairs in Si. Physical Review Letters, 2007, 99, 215503.	7.8	9
107	Intercalation of oxygen and water molecules in pentacene crystals: First-principles calculations. Physical Review B, 2007, 75, .	3.2	66
108	Role of N Defects on Thermally Induced Atomic-Scale Structural Changes in Transition-Metal Nitrides. Physical Review Letters, 2007, 99, 125503.	7.8	73

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109	Molecular dynamics simulations of stretched gold nanowires: The relative utility of different semiempirical potentials. Journal of Chemical Physics, 2007, 126, 144707.	3.0	57
110	First-principles studies of isomerization processes of silicon clusters. Physical Review B, 2007, 76, .	3.2	11
111	The Origin of Electron Mobility Enhancement in Strained MOSFETs. IEEE Electron Device Letters, 2007, 28, 1018-1020.	3.9	32
112	Hydrogen-Related Instabilities in MOS Devices Under Bias Temperature Stress. IEEE Transactions on Device and Materials Reliability, 2007, 7, 502-508.	2.0	40
113	Structure and interaction of point defects in transition-metal nitrides. Physical Review B, 2007, 76, .	3.2	78
114	Physical Mechanisms Responsible for the Abruptness of the Si-SiO2 Interface. AIP Conference Proceedings, 2007, , .	0.4	0
115	Hydrogen effects in MOS devices. Microelectronic Engineering, 2007, 84, 2344-2349.	2.4	34
116	Engineering model of a biased metalâ€“moleculeâ€“metal junction. Journal of Computational Electronics, 2007, 6, 425-430.	2.5	1
117	Effects of device aging on microelectronics radiation response and reliability. Microelectronics Reliability, 2007, 47, 1075-1085.	1.7	38
118	Hydrogen in MOSFETs â€“ A primary agent of reliability issues. Microelectronics Reliability, 2007, 47, 903-911.	1.7	54
119	DEFECT-RELATED ISSUES IN HIGH-K DIELECTRICS. , 2006, , 189-202.		1
120	Selective Nontemplated Adsorption of Organic Molecules on Nanofacets and the Role of Bonding Patterns. Physical Review Letters, 2006, 97, 156105.	7.8	65
121	Encapsulation of Floating Carbon Nanotubes inSiO2. Physical Review Letters, 2006, 97, 266805.	7.8	30
122	Thermal donor formation processes in silicon and the catalytic role of hydrogen. Applied Physics Letters, 2006, 88, 051916.	3.3	35
123	Si/SiO₂ and SiC/SiO₂ Interfaces for MOSFETs â€“ Challenges and Advances. Materials Science Forum, 2006, 527-529, 935-948.	0.3	54
124	Reactions of excess hydrogen at aSi(111)surface with H termination: First-principles calculations. Physical Review B, 2006, 74, .	3.2	10
125	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
126	Atomic-Scale Mechanisms for Low-NIEL Dopant-Type Dependent Damage in Si. IEEE Transactions on Nuclear Science, 2006, 53, 3621-3628.	2.0	14

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127	Oxygen Migration, Agglomeration, and Trapping: Key Factors for the Morphology of theSiâˆ'SiO2Interface. Physical Review Letters, 2006, 97, 116101.	7.8	42
128	Hydrogenationâˆ•deuteration of the Siâ€“SiO2 interface: Atomic-scale mechanisms and limitations. Applied Physics Letters, 2005, 86, 112107.	3.3	9
129	RelativisticNthorder muffin-tin orbital theory. Physical Review B, 2005, 71, .	3.2	0
130	Physical mechanisms of negative-bias temperature instability. Applied Physics Letters, 2005, 86, 142103.	3.3	113
131	Noncollinear magnetism of iron along the tetragonal Bain transformation. Physical Review B, 2005, 72, .	3.2	29
132	Atomic-scale mechanisms of selective adsorption and dimerization of pentacene on Si surfaces. Applied Physics Letters, 2005, 87, 233109.	3.3	23
133	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
134	Migration, incorporation, and passivation reactions of molecular hydrogen at theSiâ€“SiO2interface. Physical Review B, 2004, 70, .	3.2	48
135	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
136	Dual role of fluorine at the Siâ€“SiO2 interface. Applied Physics Letters, 2004, 85, 4950-4952.	3.3	22
137	Field-induced reactions of water molecules at Si-dielectric interfaces. Materials Research Society Symposia Proceedings, 2003, 786, 331.	0.1	3
138	Analytical Greenâ€™s-function calculation of the interlayer exchange coupling in Fe/Cr multilayers. Physical Review B, 1997, 56, R11392-R11395.	3.2	12
139	Interlayer exchange coupling in Fe/Cr multilayers. Physical Review B, 1997, 55, 11586-11592.	3.2	28
140	Effects of Device Aging on Microelectronics Radiation Response and Reliability. , 0, , .		1
141	Addition of Diquat Enhances the Electron Mobility in Various Nonâ€Fullerene Acceptor Molecules. Advanced Functional Materials, 0, , 2202954.	14.9	6