

# Geoffrey Pourtois

## List of Publications by Year in descending order

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74  
papers

2,746  
citations

361296  
20  
h-index

175177  
52  
g-index

74  
all docs

74  
docs citations

74  
times ranked

5139  
citing authors

#	ARTICLE	IF	CITATIONS
1	Strain-induced semiconductor to metal transition in the two-dimensional honeycomb structure of MoS <sub>2</sub> . Nano Research, 2012, 5, 43-48.	5.8	620
2	Bandgap opening in oxygen plasma-treated graphene. Nanotechnology, 2010, 21, 435203.	1.3	289
3	Exciton Migration in Rigid-Rod Conjugated Polymers: An Improved Förster Model. Journal of the American Chemical Society, 2005, 127, 4744-4762.	6.6	257
4	Mechanical and Electronic Properties of Thin-Film Transistors on Plastic, and Their Integration in Flexible Electronic Applications. Advanced Materials, 2016, 28, 4266-4282.	11.1	218
5	Alternating Oligo(p-phenylene vinylene)-Perylene Bisimide Copolymers: Synthesis, Photophysics, and Photovoltaic Properties of a New Class of Donor-Acceptor Materials. Journal of the American Chemical Society, 2003, 125, 8625-8638.	6.6	195
6	Photophysical Properties of Ruthenium(II) Polycyclic Aromatic Compounds: A Theoretical Insight. Journal of the American Chemical Society, 2004, 126, 683-692.	6.6	114
7	Analytical and self-consistent quantum mechanical model for the surrounding gate MOS nanowire operated in JFET mode. Journal of Computational Electronics, 2008, 7, 380-383.	1.3	87
8	Single Layer vs Bilayer Graphene: A Comparative Study of the Effects of Oxygen Plasma Treatment on Their Electronic and Optical Properties. Journal of Physical Chemistry C, 2011, 115, 16619-16624.	1.5	60
9	Capturing Wetting States in Nanopatterned Silicon. ACS Nano, 2014, 8, 885-893.	7.3	55
10	Interfaces of high-k dielectrics on GaAs: Their common features and the relationship with Fermi level pinning (Invited Paper). Microelectronic Engineering, 2009, 86, 1529-1535.	1.1	49
11	Layer-controlled epitaxy of 2D semiconductors: bridging nanoscale phenomena to wafer-scale uniformity. Nanotechnology, 2018, 29, 425602.	1.3	48
12	Titanium Silicide on Si:P With Precontact Amorphization Implantation Treatment: Contact Resistivity Approaching $1 \times 10^{-9}$ Ohm-cm <sup>2</sup> . IEEE Transactions on Electron Devices, 2016, 63, 4632-4641.	1.6	44
13	First-principles thermodynamics and defect kinetics guidelines for engineering a tailored RRAM device. Journal of Applied Physics, 2016, 119, 225107.	1.1	38
14	HfO <sub>x</sub> as RRAM material – First principles insights on the working principles. Microelectronic Engineering, 2014, 120, 13-18.	1.1	36
15	Ni fully silicided gates for 45nm CMOS applications. Microelectronic Engineering, 2005, 82, 441-448.	1.1	34
16	STM Imaging of a Heptanuclear Ruthenium(II) Dendrimer, Mono-Add Layer on Graphite. Chemistry - A European Journal, 2000, 6, 1331-1336.	1.7	33
17	Germanium: The Past and Possibly a Future Material for Microelectronics. ECS Transactions, 2007, 11, 479-493.	0.3	33
18	Topological to trivial insulating phase transition in stanene. Nano Research, 2016, 9, 774-778.	5.8	32

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19	The Vibrational Signature of the Aluminum/Polythiophene Interface. <i>Advanced Materials</i> , 1998, 10, 319-324.	11.1	25
20	Reactive molecular dynamics simulations on SiO <sub>2</sub> -coated ultra-small Si-nanowires. <i>Nanoscale</i> , 2013, 5, 719-725.	2.8	21
21	Study of the Reliability Impact of Chlorine Precursor Residues in Thin Atomic-Layer-Deposited $\text{HfO}_2$ Layers. <i>IEEE Transactions on Electron Devices</i> , 2007, 54, 752-758.	1.6	20
22	A density-functional theory simulation of the formation of Ni-doped fullerenes by ion implantation. <i>Carbon</i> , 2011, 49, 1013-1017.	5.4	20
23	Opportunities in nanometer sized Si wires for PV applications. <i>Progress in Materials Science</i> , 2013, 58, 1361-1387.	16.0	20
24	Toward an Understanding of the Electric Field-Induced Electrostatic Doping in van der Waals Heterostructures: A First-Principles Study. <i>ACS Applied Materials &amp; Interfaces</i> , 2017, 9, 7725-7734.	4.0	20
25	Atomic Layer Deposition of Ruthenium on Ruthenium Surfaces: A Theoretical Study. <i>Journal of Physical Chemistry C</i> , 2015, 119, 6592-6603.	1.5	19
26	Contact Resistance at MoS <sub>2</sub> -Based 2D Metal/Semiconductor Lateral Heterojunctions. <i>ACS Applied Nano Materials</i> , 2019, 2, 760-766.	2.4	19
27	Dielectric Response of Ta <sub>2</sub> O <sub>5</sub> , NbTaO <sub>5</sub> and Nb <sub>2</sub> O <sub>5</sub> from First-Principles Investigations. <i>ECS Transactions</i> , 2009, 19, 729-737.	0.3	17
28	(Invited) Vanadium Oxide as a Memory Material. <i>ECS Transactions</i> , 2011, 35, 233-243.	0.3	16
29	Growth and Material Characterization of Hafnium Titanates Deposited by Atomic Layer Deposition. <i>Journal of the Electrochemical Society</i> , 2009, 156, G145.	1.3	15
30	On the manifestation of phosphorus-vacancy complexes in epitaxial Si:P films. <i>Applied Physics Letters</i> , 2016, 108, .	1.5	15
31	Properties of ultrathin molybdenum films for interconnect applications. <i>Materialia</i> , 2022, 24, 101511.	1.3	15
32	Work Function Modification of Au and Ag Surfaces upon Deposition of Self-Assembled Monolayers: Influence of the Choice of the Theoretical Approach and the Thiol Decomposition Scheme. <i>ChemPhysChem</i> , 2013, 14, 2939-2946.	1.0	14
33	First-principles material modeling of solid-state electrolytes with the spinel structure. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 5399.	1.3	14
34	The Role of Nonidealities in the Scaling of MoS <sub>2</sub> FETs. <i>IEEE Transactions on Electron Devices</i> , 2018, 65, 4635-4640.	1.6	14
35	Te-induced modulation of the Mo/HfO <sub>2</sub> interface effective work function. <i>Applied Physics Letters</i> , 2008, 92, .	1.5	13
36	The Influence of the Epitaxial Growth Process Parameters on Layer Characteristics and Device Performance in Si-passivated Ge pMOSFETs. <i>ECS Transactions</i> , 2009, 19, 183-194.	0.3	13

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37	Evolution of phosphorus-vacancy clusters in epitaxial germanium. Journal of Applied Physics, 2019, 125, .	1.1	13
38	Effect of Ion Coordination on the Conformational and Electronic Structure of 3,4-Bis(alkylthio)thiophenes. European Journal of Inorganic Chemistry, 2001, 2001, 821-828.	1.0	12
39	Grain-Boundary-Induced Strain and Distortion in Epitaxial Bilayer MoS <sub>2</sub> Lattice. Journal of Physical Chemistry C, 2020, 124, 6472-6478.	1.5	12
40	Strain and ferroelectricity in wurtzite Sc <sub>x</sub> Al <sub>1-x</sub> N materials. Applied Physics Letters, 2021, 119, .	1.5	11
41	The Importance of Moisture Control for EOT Scaling of Hf-Based Dielectrics. Journal of the Electrochemical Society, 2009, 156, H416.	1.3	9
42	Crystallization resistance of barium titanate zirconate ultrathin films from aqueous CSD: a study of cause and effect. Journal of Materials Chemistry, 2009, 19, 1115.	6.7	9
43	(Invited) Boosting the On-Current of Si-Based Tunnel Field-Effect Transistors. ECS Transactions, 2010, 33, 363-372.	0.3	9
44	Selectivity Enhancement for Ruthenium Atomic Layer Deposition in Sub-50nm Nanopatterns by Diffusion and Size-Dependent Reactivity. Advanced Materials Interfaces, 2021, 8, 2100846.	1.9	9
45	Mechanisms for the Trimethylaluminum Reaction in Aluminum Oxide Atomic Layer Deposition on Sulfur Passivated Germanium. Journal of Physical Chemistry C, 2011, 115, 17523-17532.	1.5	8
46	Silicene nanoribbons on transition metal dichalcogenide substrates: Effects on electronic structure and ballistic transport. Nano Research, 2016, 9, 3394-3406.	5.8	8
47	Oxygen Defect Stability in Amorphous, <i>c</i> -Axis Aligned, and Spinel IGZO. ACS Applied Electronic Materials, 2021, 3, 4037-4046.	2.0	8
48	Hole-Doping Induced Ferromagnetism in Monolayer SnO: A First-Principles Study. ECS Transactions, 2017, 80, 339-345.	0.3	7
49	(Invited) Sub-40mV Sigma V <sub>TH</sub> Igzo nFETs in 300mm Fab. ECS Transactions, 2020, 98, 205-217.	0.3	7
50	(Invited) Stress Simulations of Fins, Wires, and Nanosheets. ECS Transactions, 2020, 98, 253-265.	0.3	7
51	Heavily phosphorus doped germanium: Strong interaction of phosphorus with vacancies and impact of tin alloying on doping activation. Journal of Applied Physics, 2019, 125, .	1.1	6
52	(Invited) Chemisorption Reaction Mechanisms for Atomic Layer Deposition of High-k Oxides on High Mobility Channels. ECS Transactions, 2010, 33, 343-353.	0.3	5
53	Some Critical Issues in Pattern Collapse Prevention and Repair. Solid State Phenomena, 0, 255, 147-151.	0.3	5
54	Source/Drain Materials for Ge nMOS Devices: Phosphorus Activation in Epitaxial Si, Ge, Ge <sub>x</sub> Sn <sub>1-x</sub> and Si <sub>y</sub> Ge <sub>1-x</sub> Sn <sub>x</sub> . ECS Journal of Solid State Science and Technology, 2020, 9, 044010.	0.9	5

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55	First-Principles Investigation of (100)Ge/Ge(Hf)O <sub>2</sub> Interfaces. ECS Transactions, 2007, 11, 471-478.	0.3	4
56	On the Evolution of Strain and Electrical Properties in As-Grown and Annealed Si:P Epitaxial Films for Source-Drain Stressor Applications. ECS Journal of Solid State Science and Technology, 2018, 7, P228-P237.	0.9	4
57	Microcanonical RT-TDDFT simulations of realistically extended devices. Journal of Chemical Physics, 2018, 149, 124701.	1.2	4
58	(Invited) First-Principles Investigation of High-k Dielectrics for Nonvolatile Memories. ECS Transactions, 2010, 33, 393-407.	0.3	3
59	Stability of Si epoxide defects in Si nanowires: a mixed reactive force field/DFT study. Physical Chemistry Chemical Physics, 2013, 15, 15091.	1.3	3
60	Ab-initio study of the segregation and electronic properties of neutral and charged B and P dopants in Si and Si/SiO <sub>2</sub> nanowires. Journal of Applied Physics, 2015, 118, 104306.	1.1	3
61	Kinetic and thermodynamic heterogeneity: an intrinsic source of variability in Cu-based RRAM memories. Journal of Computational Electronics, 2017, 16, 1011-1016.	1.3	3
62	Characterization of Highly Doped Si:P, Si:As and Si:P:As Epi Layers for Source/Drain Epitaxy. ECS Transactions, 2019, 93, 11-15.	0.3	3
63	Identifying alternative ferroelectric materials beyond Hf(Zr)O <sub>2</sub> . Applied Physics Letters, 2020, 117, 262903.	1.5	3
64	Workfunction (WF) Simulations of Ta/HfO <sub>2</sub> , Ta <sub>2</sub> C/HfO <sub>2</sub> and Ta <sub>2</sub> C/La <sub>2</sub> O <sub>3</sub> /HfO <sub>2</sub> Capped High-k Stacks. ECS Transactions, 2007, 11, 135-143.	0.3	2
65	(Invited) Aluminium Oxide Atomic Layer Deposition on Semiconductor Substrates. ECS Transactions, 2011, 41, 149-160.	0.3	2
66	Quantum simulations of electrostatics in Si cylindrical junctionless nanowire nFETs and pFETs with a homogeneous channel including strain and arbitrary crystallographic orientations. Solid-State Electronics, 2012, 71, 30-36.	0.8	2
67	Nature of electron trap states under inversion at In <sub>0.53</sub> Ga <sub>0.47</sub> As/Al <sub>2</sub> O <sub>3</sub> interfaces. Applied Physics Letters, 2017, 110, 111602.	1.5	2
68	(Invited) Probing the Intrinsic Limitations of the Contact Resistance of Metal/Semiconductor Interfaces through Atomistic Simulations. ECS Transactions, 2017, 80, 303-311.	0.3	2
69	A demonstration of donor passivation through direct formation of V <sub>As</sub> complexes in As-doped Ge <sub>1-x</sub> Sn <sub>x</sub> . Journal of Applied Physics, 2020, 127, .	1.1	2
70	Effect of Strain on the Epitaxy of B-Doped Si <sub>0.5</sub> Ge <sub>0.5</sub> Source/Drain Layers. ECS Transactions, 2021, 104, 167-179.	0.3	1
71	On the elastic tensors of ultra-thin films: A study of ruthenium. Applied Surface Science, 2022, 592, 153194.	3.1	1
72	On the Process and Material Sensitivities for High-k Based Dielectrics. ECS Transactions, 2010, 27, 693-698.	0.3	0

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73	Insights into the C Distribution in Si:C/Si:C:P and the Annealing Behavior of Si:C Layers. ECS Journal of Solid State Science and Technology, 2019, 8, P209-P216.	0.9	0
74	Point defect formation near the epitaxial Ge(001) growth surface and the impact on phosphorus doping activation. Journal of Applied Physics, 2021, 130, 125702.	1.1	0