

# Paul J Kelly

## List of Publications by Year in descending order

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108  
papers

13,887  
citations

29994

54  
h-index

28224

105  
g-index

109  
all docs

109  
docs citations

109  
times ranked

13077  
citing authors

#	ARTICLE	IF	CITATIONS
1	Doping Graphene with Metal Contacts. Physical Review Letters, 2008, 101, 026803.	2.9	2,247
2	Substrate-induced band gap in graphene on hexagonal boron nitride: <i>Ab initio</i> density functional calculations. Physical Review B, 2007, 76, .	1.1	1,292
3	First-principles study of the interaction and charge transfer between graphene and metals. Physical Review B, 2009, 79, .	1.1	1,064
4	First-principles calculation of the magnetocrystalline anisotropy energy of iron, cobalt, and nickel. Physical Review B, 1990, 41, 11919-11937.	1.1	563
5	Graphite and Graphene as Perfect Spin Filters. Physical Review Letters, 2007, 99, 176602.	2.9	415
6	Non-collinear magnetoelectronics. Physics Reports, 2006, 427, 157-255.	10.3	404
7	Theoretical study of the Si(100) surface reconstruction. Physical Review B, 1995, 51, 14504-14523.	1.1	381
8	Microscopic Theory of Atomic Diffusion Mechanisms in Silicon. Physical Review Letters, 1984, 52, 1814-1817.	2.9	318
9	Prediction and confirmation of perpendicular magnetic anisotropy in Co/Ni multilayers. Physical Review Letters, 1992, 68, 682-685.	2.9	311
10	Binding and diffusion of a Si adatom on the Si(100) surface. Physical Review Letters, 1991, 66, 1729-1732.	2.9	291
11	Thermal Spin-Transfer Torque in Magnetoelectronic Devices. Physical Review Letters, 2007, 99, 066603.	2.9	261
12	Magnetocrystalline anisotropy and orbital moments in transition-metal compounds. Physical Review B, 1991, 44, 12054-12057.	1.1	230
13	Spin torques in ferromagnetic/normal-metal structures. Physical Review B, 2002, 65, .	1.1	224
14	Large Orbital-Moment Contribution to 5f Band Magnetism. Physical Review Letters, 1983, 51, 1708-1711.	2.9	206
15	First-principles study of magnetization relaxation enhancement and spin transfer in thin magnetic films. Physical Review B, 2005, 71, .	1.1	197
16	Theoretical prediction of perfect spin filtering at interfaces between close-packed surfaces of Ni or Co and graphite or graphene. Physical Review B, 2008, 78, .	1.1	186
17	Giant Room Temperature Interface Spin Hall and Inverse Spin Hall Effects. Physical Review Letters, 2016, 116, 196602.	2.9	181
18	Magnetic anisotropy of a free-standing Co monolayer and of multilayers which contain Co monolayers. Physical Review B, 1994, 50, 9989-10003.	1.1	177

#	ARTICLE	IF	CITATIONS
19	Adsorption of Al on Si(100): A surface polymerization reaction. Physical Review Letters, 1993, 70, 2786-2789.	2.9	171
20	Giant Magnetoresistance without Defect Scattering. Physical Review Letters, 1995, 74, 586-589.	2.9	168
21	Conductance calculations for quantum wires and interfaces: Mode matching and Green's functions. Physical Review B, 2005, 72, .	1.1	168
22	Interface Enhancement of Gilbert Damping from First Principles. Physical Review Letters, 2014, 113, 207202.	2.9	168
23	First-principles calculation of the magnetic anisotropy energy of (Co)n/(X)m multilayers. Physical Review B, 1990, 42, 7270-7273.	1.1	163
24	Thermoelectric effects in magnetic nanostructures. Physical Review B, 2009, 79, .	1.1	160
25	Ab Initio Calculation of the Gilbert Damping Parameter via the Linear Response Formalism. Physical Review Letters, 2011, 107, 066603.	2.9	153
26	Microscopic Theory of Impurity-Defect Reactions and Impurity Diffusion in Silicon. Physical Review Letters, 1985, 54, 360-363.	2.9	146
27	Ab Initio Calculation of the Electronic and Optical Excitations in Polythiophene: Effects of Intra- and Interchain Screening. Physical Review Letters, 1999, 83, 4413-4416.	2.9	142
28	Theoretical Prediction of the Structure of Insulating YH <sub>3</sub> . Physical Review Letters, 1997, 78, 1315-1318.	2.9	135
29	CaB <sub>6</sub> : A New Semiconducting Material for Spin Electronics. Physical Review Letters, 2001, 87, 016401.	2.9	133
30	Polarity-induced oxygen vacancies at LaAlO <sub>3</sub> /SrTiO <sub>3</sub> interface. Physical Review B, 2010, 82, .	2.9	124
31	Electrostatic Doping of Graphene through Ultrathin Hexagonal Boron Nitride Films. Nano Letters, 2011, 11, 4631-4635.	4.5	118
32	Unified First-Principles Study of Gilbert Damping, Spin-Flip Diffusion, and Resistivity in Transition Metal Alloys. Physical Review Letters, 2010, 105, 236601.	2.9	111
33	Optical transmission spectroscopy of switchable yttrium hydride films. Physical Review B, 1998, 57, 4943-4949.	1.1	108
34	Interface resistance of disordered magnetic multilayers. Physical Review B, 2001, 63, .	1.1	107
35	Nonlinear screening of charges induced in graphene by metal contacts. Physical Review B, 2010, 82, .	1.1	105
36	First-principles scattering matrices for spin transport. Physical Review B, 2006, 73, .	1.1	104

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37	Dynamics and Nucleation of Si Ad-dimers on the Si(100) Surface. Physical Review Letters, 1996, 76, 2362-2365.	2.9	101
38	Band gaps in incommensurable graphene on hexagonal boron nitride. Physical Review B, 2014, 89, .	1.1	97
39	Ballistic electron transport through magnetic domain walls. Physical Review B, 1999, 59, 138-141.	1.1	95
40	Interface resistances of magnetic multilayers. Physical Review B, 1997, 56, 10805-10808.	1.1	94
41	Schottky barriers at hexagonal boron nitride/metal interfaces: A first-principles study. Physical Review B, 2014, 90, .	1.1	87
42	Ballistic transport and electronic structure. Physical Review B, 1998, 57, 8907-8926.	1.1	83
43	Inversion of Spin Signal and Spin Filtering in Ferromagnet   Hexagonal Boron Nitride-Graphene van der Waals Heterostructures. Scientific Reports, 2016, 6, 21168.	1.6	79
44	Electronic-structureâ€“induced reconstruction and magnetic ordering at the LaAlO <sub>3</sub>   SrTiO <sub>3</sub> interface. Europhysics Letters, 2008, 84, 27001.	0.7	74
45	Perpendicular magnetic anisotropy of multilayers: recent insights. Journal of Magnetism and Magnetic Materials, 1995, 148, 118-124.	1.0	72
46	Parameter-Free Quasiparticle Calculations for YH <sub>3</sub> . Physical Review Letters, 2000, 85, 2989-2992.	2.9	72
47	Ni(111)   graphene-BN junctions as ideal spin injectors. Physical Review B, 2011, 84, .	1.1	69
48	First-principles calculations of magnetization relaxation in pure Fe, Co, and Ni with frozen thermal lattice disorder. Physical Review B, 2011, 84, .	1.1	67
49	Hard x-ray photoemission and density functional theory study of the internal electric field in SrTiO <sub>3</sub> / LaAlO <sub>3</sub> oxide heterostructures. Physical Review B, 2013, 87, .	1.1	64
50	Spin-Dependent Transparency of Ferromagnet/Superconductor Interfaces. Physical Review Letters, 2002, 89, 166603.	2.9	63
51	Spin injection through an Fe/InAs interface. Physical Review B, 2003, 67, .	1.1	63
52	Greenâ€™s-matrix calculation of total energies of point defects in silicon. Physical Review B, 1992, 45, 6543-6563.	1.1	62
53	Electronic structure and ground-state properties of the actinide dioxides. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 1189.	1.1	57
54	Direct method for calculating temperature-dependent transport properties. Physical Review B, 2015, 91, .	1.1	57

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55	Disorder Dependence of Interface Spin Memory Loss. <i>Physical Review Letters</i> , 2020, 124, 087702.	2.9	57
56	Influence of roughness and disorder on tunneling magnetoresistance. <i>Physical Review B</i> , 2006, 73, .	1.1	56
57	Magnetocrystalline anisotropy of YCo <sub>5</sub> and related RECo <sub>5</sub> compounds. <i>Physical Review B</i> , 1996, 53, 14415-14433.	1.1	55
58	Ab initio prediction of the electronic and optical excitations in polythiophene: Isolated chains versus bulk polymer. <i>Physical Review B</i> , 2000, 61, 15817-15826.	1.1	47
59	Calculating scattering matrices by wave function matching. <i>Physica Status Solidi (B): Basic Research</i> , 2008, 245, 623-640.	0.7	46
60	Calculating the transport properties of magnetic materials from first principles including thermal and alloy disorder, noncollinearity, and spin-orbit coupling. <i>Physical Review B</i> , 2018, 97, .	1.1	44
61	Structure and properties of polymers calculated by Ab initio molecular dynamics. <i>Synthetic Metals</i> , 1993, 57, 4243-4248.	2.1	40
62	Phonon spectrum of YH <sub>3</sub> : Evidence for a broken symmetry structure. <i>Physical Review B</i> , 2001, 63, .	1.1	38
63	On the cohesive energy and charge density of uranium dioxide. <i>Solid State Communications</i> , 1983, 45, 689-692.	0.9	37
64	Prediction of thickness limits of ideal polar ultrathin films. <i>Physical Review B</i> , 2012, 85, .	1.1	36
65	Gilbert Damping in Noncollinear Ferromagnets. <i>Physical Review Letters</i> , 2014, 113, 266603.	2.9	35
66	Invariance of Germanene on $Z_2$ MoS <sub>2</sub> First Principles. <i>Physical Review Letters</i> , 2016, 116, 256805.	2.9	35
67	Scattering theory of interface resistance in magnetic multilayers. <i>Journal Physics D: Applied Physics</i> , 2002, 35, 2410-2414.	1.3	34
68	Theory of electronically stimulated defect migration in semiconductors. <i>Physical Review B</i> , 1984, 30, 2260-2262.	1.1	33
69	Field-effect doping of graphene in metal-graphene heterostructures: A model based upon first-principles calculations. <i>Physical Review B</i> , 2013, 87, .	1.1	33
70	Tuning Ferromagnetism at Interfaces between Insulating Perovskite Oxides. <i>Physical Review Letters</i> , 2014, 113, 127201.	2.9	33
71	Parameter-free calculation of single-particle electronic excitations in YH <sub>3</sub> . <i>Physical Review B</i> , 2002, 66, .	1.1	31
72	Orientation-Dependent Transparency of Metallic Interfaces. <i>Physical Review Letters</i> , 2006, 96, 176602.	2.9	27

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73	Structural and dynamical properties of YH <sub>3</sub> . Physical Review B, 2003, 68, .	1.1	26
74	Dynamic Ferromagnetic Proximity Effect in Photoexcited Semiconductors. Physical Review Letters, 2004, 92, 126601.	2.9	26
75	Calculating spin transport properties from first principles: Spin currents. Physical Review B, 2019, 99, .	1.1	25
76	Cohesive properties of CaF <sub>2</sub> and UO <sub>2</sub> in the atomic sphere approximation. Journal of Physics C: Solid State Physics, 1980, 13, L939-L945.	1.5	24
77	Large potential steps at weakly interacting metal-insulator interfaces. Physical Review B, 2014, 90, .	1.1	24
78	Comment on State-tracking first-principles determination of magnetocrystalline anisotropy. Physical Review Letters, 1993, 71, 2165-2165.	2.9	19
79	Aluminum on Si(100): Growth and structure of the first layer. Journal of Vacuum Science & Technology an Official Journal of the American Vacuum Society B, Microelectronics Processing and Phenomena, 1994, 12, 2705.	1.6	19
80	Spin-Orbit-Coupling-Induced Domain-Wall Resistance in Diffusive Ferromagnets. Physical Review Letters, 2012, 109, 267201.	2.9	19
81	Kelly, Dekker, and Stumpf Reply:. Physical Review Letters, 1997, 79, 2921-2921.	2.9	18
82	Spin accumulation and decay in magnetic Schottky barriers. Physical Review B, 2005, 72, .	1.1	17
83	Itinerant ferromagnetism in $p$ -doped monolayers of $\text{MoS}_2$ . Physical Review B, 2019, 99, .	1.1	16
84	Scattering theory of perpendicular transport in metallic multilayers (invited). Journal of Applied Physics, 1994, 75, 6704-6708.	1.1	15
85	Spin-orbit-coupling induced torque in ballistic domain walls: Equivalence of charge-pumping and nonequilibrium magnetization formalisms. Physical Review B, 2016, 93, .	1.1	15
86	Semiclassical concepts in magnetoelectronics. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2001, 84, 31-36.	1.7	11
87	Spin-Flip Diffusion Length in $d$ -Transition Metal Elements: A First-Principles Benchmark. Physical Review Letters, 2021, 126, 196601.	2.9	10
88	Electronic structure and ionicity of actinide dioxides. Journal De Physique Colloque, 1979, 40, C4-184-C4-186.	0.2	10
89	Electronic properties of expanded cesium. Physical Review B, 1986, 33, 5284-5293.	1.1	9
90	DFT study of itinerant ferromagnetism in $p$ -doped monolayers of $\text{MoS}_2$ . Physical Review B, 2019, 100, .	1.1	9

#	ARTICLE	IF	CITATIONS
91	MAGNETIC ANISOTROPY IN Fe, Co AND Ni. Journal De Physique Colloque, 1988, 49, C8-93-C8-94.	0.2	9
92	Ab-initio calculation of quasi-particle bandstructure, exciton binding energies and dielectric properties of polythiophene. Synthetic Metals, 1999, 101, 333-334.	2.1	8
93	Ballistic giant magnetoresistance. Journal of Magnetism and Magnetic Materials, 1996, 156, 385-386.	1.0	7
94	Crystalline CoFeB/Graphite Interfaces for Carbon Spintronics Fabricated by Solid Phase Epitaxy. Advanced Functional Materials, 2013, 23, 4933-4940.	7.8	7
95	Excitons in conjugated polymers from first principles. Computer Physics Communications, 2002, 147, 331-334.	3.0	6
96	Spin transport at finite temperatures: A first-principles study for $\langle \text{mml:math} \text{xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mtext} \rangle \text{ferromagnetic} \langle \text{mml:mtext} \rangle \langle \text{mml:mo} \rangle   \langle \text{mml:mo} \rangle \langle \text{mml:mtext} \rangle \text{metal} \langle \text{mml:mtext} \rangle \text{interfaces}$ . Physical Review B, 2021, 104, .	1.0	6
97	Giant magnetoresistance from first principles. Journal of Magnetism and Magnetic Materials, 1995, 140-144, 503-504.	1.0	5
98	Mesoscopic aspects of the giant magnetoresistance. Journal of Magnetism and Magnetic Materials, 1995, 151, 369-373.	1.0	4
99	Many-body solid-state methods for the calculation of the electronic and optical properties of conjugated polymers. Synthetic Metals, 2001, 119, 209-210.	2.1	4
100	Calculating the spin memory loss at Cu   metal interfaces from first principles. Physical Review B, 2022, 106, .	1.1	4
101	Fully resolved currents from quantum transport calculations. Physical Review B, 2021, 103, .	1.1	3
102	Giant Magnetoresistance and Electronic Structure. Materials Research Society Symposia Proceedings, 1995, 384, 305.	0.1	2
103	Spin-injection through an Fe/InAs interface. Physica Status Solidi A, 2003, 196, 25-28.	1.7	2
104	Spin Hall effect in a thin Pt film. Physical Review B, 2021, 104, .	1.1	2
105	First-Principles Calculation of the Magnetocrystalline Anisotropy Energy of ConPdm Multilayers. NATO ASI Series Series B: Physics, 1991, , 185-190.	0.2	1
106	Defect Structure and Dynamics in Silicon. Materials Research Society Symposia Proceedings, 1985, 63, 7.	0.1	0
107	Chapter Two Magnetic Nanostructures: Currents and Dynamics. Handbook of Magnetic Materials, 2007, , 123-148.	0.6	0
108	Disordered Regions in Crystalline Silicon at High Temperatures. , 1985, , 265-273.		0