Paul J Kelly

List of Publications by Year
in descending order

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	Calculating the spin memory loss at Cu|metal interfaces from first principles. Physical Review B, 2022, 106, .	1.1	4
2	Fully resolved currents from quantum transport calculations. Physical Review B, 2021, 103, .	1.1	3
3	Spin-Flip Diffusion Length in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>5</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math> Transition Metal Elements: A First-Principles Benchmark. Physical Review Letters, 2021, 126, 196601.	2.9	10
4	Spin transport at finite temperatures: A first-principles study for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mtext>ferromagnetic</mml:mtext><mml:mo>|</mml:mo><mml:mtext>no</mml:mtext> interfaces. Physical Review B, 2021, 104, .	1.1	6
5	Spin Hall effect in a thin Pt film. Physical Review B, 2021, 104, .	1.1	2
6	Disorder Dependence of Interface Spin Memory Loss. Physical Review Letters, 2020, 124, 087702.	2.9	57
7	Itinerant ferromagnetism in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi></mml:math> -doped monolayers of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2019, 99, .	1.1	16
8	Calculating spin transport properties from first principles: Spin currents. Physical Review B, 2019, 99, .	1.1	25
9	DFT study of itinerant ferromagnetism in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi></mml:math> -doped monolayers of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2019, 100, .	1.1	9
10	Calculating the transport properties of magnetic materials from first principles including thermal and alloy disorder, noncollinearity, and spin-orbit coupling. Physical Review B, 2018, 97, .	1.1	44
11	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
12	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
13	Giant Room Temperature Interface Spin Hall and Inverse Spin Hall Effects. Physical Review Letters, 2016, 116, 196602.	2.9	181
14	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="double-struck">Z</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>Invariance of Germanene on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>MoS</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow> First Principles. Physical Review Letters, 2016, 116, 256805.	2.9	35
15	Direct method for calculating temperature-dependent transport properties. Physical Review B, 2015, 91, .	1.1	57
16	Gilbert Damping in Noncollinear Ferromagnets. Physical Review Letters, 2014, 113, 266603.	2.9	35
17	Tuning Ferromagnetism at Interfaces between Insulating Perovskite Oxides. Physical Review Letters, 2014, 113, 127201.	2.9	33
18	Schottky barriers at hexagonal boron nitride/metal interfaces: A first-principles study. Physical Review B, 2014, 90, .	1.1	87

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19	Large potential steps at weakly interacting metal-insulator interfaces. Physical Review B, 2014, 90, .	1.1	24
20	Interface Enhancement of Gilbert Damping from First Principles. Physical Review Letters, 2014, 113, 207202.	2.9	168
21	Band gaps in incommensurable graphene on hexagonal boron nitride. Physical Review B, 2014, 89, .	1.1	97
22	Hard x-ray photoemission and density functional theory study of the internal electric field in SrTiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>/LaAlO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>3</mml:mn></mml:msub></mml:math>oxide heterostructures. Physical Review B, 2013, 87, .	1.1	64
23	Field-effect doping of graphene in metal<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo>|</mml:mo></mml:math>dielectric<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo>|</mml:mo></mml:math>graphene heterostructures: A model based upon first-principles calculations. Physical Review B, 2013, 87, .	1.1	33
24	Crystalline CoFeB/Graphite Interfaces for Carbon Spintronics Fabricated by Solid Phase Epitaxy. Advanced Functional Materials, 2013, 23, 4933-4940.	7.8	7
25	Prediction of thickness limits of ideal polar ultrathin films. Physical Review B, 2012, 85, .	1.1	36
26	Spin-Orbit-Coupling-Induced Domain-Wall Resistance in Diffusive Ferromagnets. Physical Review Letters, 2012, 109, 267201.	2.9	19
27	<i>AbÂInitio</i>Calculation of the Gilbert Damping Parameter via the Linear Response Formalism. Physical Review Letters, 2011, 107, 066603.	2.9	153
28	Electrostatic Doping of Graphene through Ultrathin Hexagonal Boron Nitride Films. Nano Letters, 2011, 11, 4631-4635.	4.5	118
29	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
30	Ni(111)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo>|</mml:mo></mml:math>graphene<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo>|</mml:mo><mml:mi>h</mml:mi></mml:mrow></mml:math>-BN junctions as ideal spin injectors. Physical Review B, 2011, 84, .	1.1	69
31	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
32	Nonlinear screening of charges induced in graphene by metal contacts. Physical Review B, 2010, 82, .	1.1	105
33	Polarity-induced oxygen vacancies at<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaAlO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mm Physical Review B, 2010, 82, .	1.1	124
34	Thermoelectric effects in magnetic nanostructures. Physical Review B, 2009, 79, .	1.1	160
35	First-principles study of the interaction and charge transfer between graphene and metals. Physical Review B, 2009, 79, .	1.1	1,064
36	Calculating scattering matrices by wave function matching. Physica Status Solidi (B): Basic Research, 2008, 245, 623-640.	0.7	46

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37	Doping Graphene with Metal Contacts. Physical Review Letters, 2008, 101, 026803.	2.9	2,247
38	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
39	Electronic-structureâ€“induced reconstruction and magnetic ordering at the LaAlO ₃ |SrTiO ₃ interface. Europhysics Letters, 2008, 84, 27001.	0.7	74
40	Chapter Two Magnetic Nanostructures: Currents and Dynamics. Handbook of Magnetic Materials, 2007, , 123-148.	0.6	0
41	Substrate-induced band gap in graphene on hexagonal boron nitride:Ab initiodensity functional calculations. Physical Review B, 2007, 76, .	1.1	1,292
42	Graphite and Graphene as Perfect Spin Filters. Physical Review Letters, 2007, 99, 176602.	2.9	415
43	Thermal Spin-Transfer Torque in Magnetoelectronic Devices. Physical Review Letters, 2007, 99, 066603.	2.9	261
44	Influence of roughness and disorder on tunneling magnetoresistance. Physical Review B, 2006, 73, .	1.1	56
45	Non-collinear magnetoelectronics. Physics Reports, 2006, 427, 157-255.	10.3	404
46	Orientation-Dependent Transparency of Metallic Interfaces. Physical Review Letters, 2006, 96, 176602.	2.9	27
47	First-principles scattering matrices for spin transport. Physical Review B, 2006, 73, .	1.1	104
48	Spin accumulation and decay in magnetic Schottky barriers. Physical Review B, 2005, 72, .	1.1	17
49	First-principles study of magnetization relaxation enhancement and spin transfer in thin magnetic films. Physical Review B, 2005, 71, .	1.1	197
50	Conductance calculations for quantum wires and interfaces: Mode matching and Greenâ€™s functions. Physical Review B, 2005, 72, .	1.1	168
51	Dynamic Ferromagnetic Proximity Effect in Photoexcited Semiconductors. Physical Review Letters, 2004, 92, 126601.	2.9	26
52	Spin-injection through an Fe/InAs interface. Physica Status Solidi A, 2003, 196, 25-28.	1.7	2
53	Spin injection through an Fe/InAs interface. Physical Review B, 2003, 67, .	1.1	63
54	Structural and dynamical properties ofYH3. Physical Review B, 2003, 68, .	1.1	26

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55	Parameter-free calculation of single-particle electronic excitations inYH3. Physical Review B, 2002, 66, .	1.1	31
56	Spin-Dependent Transparency of Ferromagnet/Superconductor Interfaces. Physical Review Letters, 2002, 89, 166603.	2.9	63
57	Scattering theory of interface resistance in magnetic multilayers. Journal Physics D: Applied Physics, 2002, 35, 2410-2414.	1.3	34
58	Spin torques in ferromagnetic/normal-metal structures. Physical Review B, 2002, 65, .	1.1	224
59	Excitons in conjugated polymers from first principles. Computer Physics Communications, 2002, 147, 331-334.	3.0	6
60	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
61	Phonon spectrum ofYH3:â€ƒEvidence for a broken symmetry structure. Physical Review B, 2001, 63, .	1.1	38
62	Semiclassical concepts in magnetoelectronics. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2001, 84, 31-36.	1.7	11
63	CaB6: A New Semiconducting Material for Spin Electronics. Physical Review Letters, 2001, 87, 016401.	2.9	133
64	Interface resistance of disordered magnetic multilayers. Physical Review B, 2001, 63, .	1.1	107
65	Parameter-Free Quasiparticle Calculations forYH3. Physical Review Letters, 2000, 85, 2989-2992.	2.9	72
66	Ab initioprediction of the electronic and optical excitations in polythiophene: Isolated chains versus bulk polymer. Physical Review B, 2000, 61, 15817-15826.	1.1	47
67	Ab InitioCalculation of the Electronic and Optical Excitations in Polythiophene: Effects of Intra- and Interchain Screening. Physical Review Letters, 1999, 83, 4413-4416.	2.9	142
68	Ballistic electron transport through magnetic domain walls. Physical Review B, 1999, 59, 138-141.	1.1	95
69	Ab-initio calculation of quasi-particle bandstructure, exciton binding energies and dielectric properties of polythiophene. Synthetic Metals, 1999, 101, 333-334.	2.1	8
70	Ballistic transport and electronic structure. Physical Review B, 1998, 57, 8907-8926.	1.1	83
71	Optical transmission spectroscopy of switchable yttrium hydride films. Physical Review B, 1998, 57, 4943-4949.	1.1	108
72	Kelly, Dekker, and Stumpf Reply:. Physical Review Letters, 1997, 79, 2921-2921.	2.9	18

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73	Interface resistances of magnetic multilayers. Physical Review B, 1997, 56, 10805-10808.	1.1	94
74	Theoretical Prediction of the Structure of InsulatingYH3. Physical Review Letters, 1997, 78, 1315-1318.	2.9	135
75	Ballistic giant magnetoresistance. Journal of Magnetism and Magnetic Materials, 1996, 156, 385-386.	1.0	7
76	Magnetocrystalline anisotropy of YCo5and related RECo5compounds. Physical Review B, 1996, 53, 14415-14433.	1.1	55
77	Dynamics and Nucleation of Si Ad-dimers on the Si(100) Surface. Physical Review Letters, 1996, 76, 2362-2365.	2.9	101
78	Giant Magnetoresistance and Electronic Structure. Materials Research Society Symposia Proceedings, 1995, 384, 305.	0.1	2
79	Perpendicular magnetic anisotropy of multilayers: recent insights. Journal of Magnetism and Magnetic Materials, 1995, 148, 118-124.	1.0	72
80	Mesoscopic aspects of the giant magnetoresistance. Journal of Magnetism and Magnetic Materials, 1995, 151, 369-373.	1.0	4
81	Giant magnetoresistance from first principles. Journal of Magnetism and Magnetic Materials, 1995, 140-144, 503-504.	1.0	5
82	Theoretical study of the Si(100) surface reconstruction. Physical Review B, 1995, 51, 14504-14523.	1.1	381
83	Giant Magnetoresistance without Defect Scattering. Physical Review Letters, 1995, 74, 586-589.	2.9	168
84	Scattering theory of perpendicular transport in metallic multilayers (invited). Journal of Applied Physics, 1994, 75, 6704-6708.	1.1	15
85	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
86	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
87	Comment on State-tracking first-principles determination of magnetocrystalline anistropy. Physical Review Letters, 1993, 71, 2165-2165.	2.9	19
88	Structure and properties of polymers calculated by Ab initio molecular dynamics. Synthetic Metals, 1993, 57, 4243-4248.	2.1	40
89	Adsorption of Al on Si(100): A surface polymerization reaction. Physical Review Letters, 1993, 70, 2786-2789.	2.9	171
90	Greenâ€™s-matrix calculation of total energies of point defects in silicon. Physical Review B, 1992, 45, 6543-6563.	1.1	62

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91	Prediction and confirmation of perpendicular magnetic anisotropy in Co/Ni multilayers. Physical Review Letters, 1992, 68, 682-685.	2.9	311
92	Magnetocrystalline anisotropy and orbital moments in transition-metal compounds. Physical Review B, 1991, 44, 12054-12057.	1.1	230
93	Binding and diffusion of a Si adatom on the Si(100) surface. Physical Review Letters, 1991, 66, 1729-1732.	2.9	291
94	First-Principles Calculation of the Magnetocrystalline Anisotropy Energy of ConPdm Multilayers. NATO ASI Series Series B: Physics, 1991, , 185-190.	0.2	1
95	First-principles calculation of the magnetic anisotropy energy of (Co)n/(X)mmultilayers. Physical Review B, 1990, 42, 7270-7273.	1.1	163
96	First-principles calculation of the magnetocrystalline anisotropy energy of iron, cobalt, and nickel. Physical Review B, 1990, 41, 11919-11937.	1.1	563
97	MAGNETIC ANISOTROPY IN Fe, Co AND Ni. Journal De Physique Colloque, 1988, 49, C8-93-C8-94.	0.2	9
98	Electronic structure and ground-state properties of the actinide dioxides. Journal of the Chemical Society, Faraday Transactions 2, 1987, 83, 1189.	1.1	57
99	Electronic properties of expanded cesium. Physical Review B, 1986, 33, 5284-5293.	1.1	9
100	Defect Structure and Dynamics in Silicon. Materials Research Society Symposia Proceedings, 1985, 63, 7.	0.1	0
101	Microscopic Theory of Impurity-Defect Reactions and Impurity Diffusion in Silicon. Physical Review Letters, 1985, 54, 360-363.	2.9	146
102	Disordered Regions in Crystalline Silicon at High Temperatures. , 1985, , 265-273.		0
103	Microscopic Theory of Atomic Diffusion Mechanisms in Silicon. Physical Review Letters, 1984, 52, 1814-1817.	2.9	318
104	Theory of electronically stimulated defect migration in semiconductors. Physical Review B, 1984, 30, 2260-2262.	1.1	33
105	On the cohesive energy and charge density of uranium dioxide. Solid State Communications, 1983, 45, 689-692.	0.9	37
106	Large Orbital-Moment Contribution to5fBand Magnetism. Physical Review Letters, 1983, 51, 1708-1711.	2.9	206
107	Cohesive properties of CaF2and UO2in the atomic sphere approximation. Journal of Physics C: Solid State Physics, 1980, 13, L939-L945.	1.5	24
108	Electronic structure and ionicity of actinide dioxides. Journal De Physique Colloque, 1979, 40, C4-184-C4-186.	0.2	10