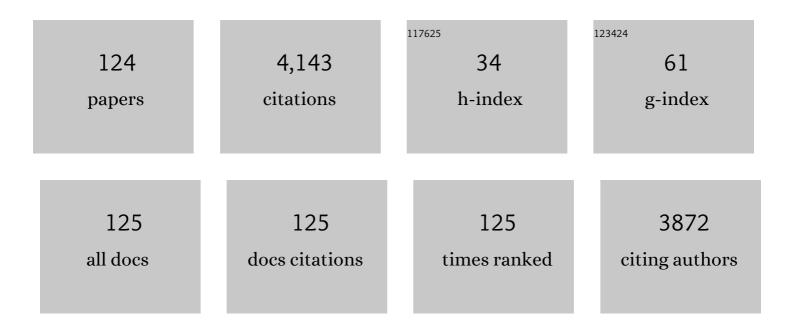
List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Rydberg entangling gates in silicon. Physical Review Research, 2021, 3, .	3.6	4
2	Excited states of a phosphorus pair in silicon: Combining valley-orbital interaction and electron-electron interactions. Physical Review B, 2021, 104, .	3.2	3
3	Multihole models for deterministically placed acceptor arrays in silicon. Physical Review B, 2021, 104, .	3.2	1
4	Linear combination of atomic orbitals model for deterministically placed acceptor arrays in silicon. Physical Review B, 2020, 101, .	3.2	5
5	Topological phases of a dimerized Fermi–Hubbard model for semiconductor nano-lattices. Npj Quantum Information, 2020, 6, .	6.7	27
6	Optically controlled entangling gates in randomly doped silicon. Physical Review B, 2019, 100, .	3.2	2
7	Excited states of defect linear arrays in silicon: A first-principles study based on hydrogen cluster analogs. Physical Review B, 2018, 97, .	3.2	4
8	Two- to three-dimensional crossover in a dense electron liquid in silicon. Physical Review B, 2018, 97, .	3.2	5
9	Controlling electronic access to the spin excitations of a single molecule in a tunnel junction. Nanoscale, 2017, 9, 4053-4057.	5.6	2
10	Exact location of dopants below the Si(001):H surface from scanning tunneling microscopy and density functional theory. Physical Review B, 2017, 95, .	3.2	10
11	Extended Hubbard model for mesoscopic transport in donor arrays in silicon. Physical Review B, 2017, 96, .	3.2	20
12	Optical response from terahertz to visible light of electronuclear transitions inLiYF4:Ho3+. Physical Review B, 2016, 94, .	3.2	10
13	Sub-molecular modulation of a 4f driven Kondo resonance by surface-induced asymmetry. Nature Communications, 2016, 7, 12785.	12.8	32
14	Tunable magnetoresistance in an asymmetrically coupled single-molecule junction. Nature Nanotechnology, 2015, 10, 259-263.	31.5	56
15	High-temperature antiferromagnetism in molecular semiconductor thin films and nanostructures. Nature Communications, 2014, 5, 3079.	12.8	76
16	Potential for spin-based information processing in a thin-film molecular semiconductor. Nature, 2013, 503, 504-508.	27.8	236
17	<mml:math <br="" xmlns:mml="http://www.w3.org/1998/Math/MathML">display="inline"&gt;<mml:mi>p</mml:mi></mml:math> -orbital nanomagnetism in an organic chain magnet. Physical Review B, 2013, 88, .	3.2	11
18	Switching and propagation of magnetoplasmon polaritons in magnetic slot waveguides and cavities. Physical Review B, 2013, 88, .	3.2	15

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19	Magnetic properties of copper hexadecaphthalocyanine (F16CuPc) thin films and powders. Journal of Applied Physics, 2013, 113, 013914.	2.5	17
20	Half-filled orbital and unconventional geometry of a common dopant in Si(001). Physical Review B, 2013, 88, .	3.2	2
21	Electronic structure and exchange interactions in cobalt-phthalocyanine chains. Physical Review B, 2013, 88, .	3.2	31
22	Suitability of chromium phthalocyanines to test Haldane's conjecture: First-principles calculations. Physical Review B, 2013, 88, .	3.2	8
23	Cavity-enhanced magneto-plasmonic effects. Proceedings of SPIE, 2012, , .	0.8	0
24	Scanning Tunneling Microscopy Contrast Mechanisms for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"&gt;<mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub>. Physical Review Letters, 2012, 109, 156105.</mml:math 	7.8	38
25	Contribution of spin pairs to the magnetic response in a dilute dipolar ferromagnet. Physical Review B, 2012, 86, .	3.2	5
26	Theoretical modeling of the electronic structure and exchange interactions in Cu(II)Pc. Journal of Physics: Conference Series, 2012, 391, 012119.	0.4	1
27	Spin-Based Diagnostic of Nanostructure in Copper Phthalocyanine–C <sub>60</sub> Solar Cell Blends. ACS Nano, 2012, 6, 10808-10815.	14.6	24
28	Theoretical modeling of the electronic structure and exchange interactions in a Cu(II)Pc one-dimensional chain. Physical Review B, 2011, 84, .	3.2	22
29	A multiconfigurational time-dependent Hartree-Fock method for excited electronic states. I. General formalism and application to open-shell states. Journal of Chemical Physics, 2011, 134, 244101.	3.0	48
30	A multiconfigurational time-dependent Hartree-Fock method for excited electronic states. II. Coulomb interaction effects in single conjugated polymer chains. Journal of Chemical Physics, 2011, 134, 244102.	3.0	18
31	Analog of Rabi oscillations in resonant electron-ion systems. Journal of Chemical Physics, 2011, 134, 194105.	3.0	8
32	Modelling non-adiabatic processes using correlated electron-ion dynamics. European Physical Journal B, 2010, 77, 305-329.	1.5	33
33	Separation-dependent localization in a two-impurity spin-boson model. Physical Review B, 2010, 81, .	3.2	28
34	Electron traps and their effect on the surface chemistry of TiO <sub>2</sub> (110). Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 2391-2396.	7.1	264
35	Ultralong Copper Phthalocyanine Nanowires with New Crystal Structure and Broad Optical Absorption. ACS Nano, 2010, 4, 3921-3926.	14.6	47
36	Hydroxyl vacancies in single-walled aluminosilicate and aluminogermanate nanotubes. Journal of Physics Condensed Matter, 2009, 21, 195301.	1.8	20

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37	Long-lived spin entanglement induced by a spatially correlated thermal bath. Physical Review A, 2009, 80, .	2.5	43
38	Correlated electron-ion dynamics in metallic systems. Computational Materials Science, 2008, 44, 16-20.	3.0	12
39	Local entanglement of multidimensional continuous-variable systems. Physical Review A, 2008, 78, .	2.5	Ο
40	Structure-dependent exchange in the organic magnets Cu(II)Pc and Mn(II)Pc. Physical Review B, 2008, 77, .	3.2	38
41	Exchange between deep donors in semiconductors: A quantum defect approach. Physical Review B, 2008, 77, .	3.2	7
42	Robust nonadiabatic molecular dynamics for metals and insulators. Journal of Chemical Physics, 2007, 127, 214104.	3.0	21
43	Quantum Projection in an Ising Spin Liquid. Physical Review Letters, 2007, 99, 057203.	7.8	12
44	Entanglement in general two-mode continuous-variable states: Local approach and mapping to a two-qubit system. Physical Review A, 2007, 76, .	2.5	1
45	Configuration-space location of the entanglement between two subsystems. Physical Review A, 2007, 75, .	2.5	3
46	Molecular Thin Films: A New Type of Magnetic Switch. Advanced Materials, 2007, 19, 3618-3622.	21.0	133
47	The transfer of energy between electrons and ions in solids. Reports on Progress in Physics, 2006, 69, 1195-1234.	20.1	77
48	Hofer and Fisher Reply:. Physical Review Letters, 2006, 96, .	7.8	33
49	Quantum communication in spin systems with long-range interactions. Physical Review A, 2006, 74, .	2.5	53
50	Vibrational inelastic scattering effects in molecular electronics. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 8826-8831.	7.1	26
51	Correlated electron–ion dynamics: the excitation of atomic motion by energetic electrons. Journal of Physics Condensed Matter, 2005, 17, 4793-4812.	1.8	57
52	Open-boundary Ehrenfest molecular dynamics: towards a model of current induced heating in nanowires. Journal of Physics Condensed Matter, 2004, 16, L65-L72.	1.8	32
53	Power dissipation in nanoscale conductors: classical, semi-classical and quantum dynamics. Journal of Physics Condensed Matter, 2004, 16, 3609-3622.	1.8	79
54	Avoiding entanglement loss when two-qubit quantum gates are controlled by electronic excitation. Journal of Physics Condensed Matter, 2004, 16, 2757-2772.	1.8	15

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55	Beyond Ehrenfest: correlated non-adiabatic molecular dynamics. Journal of Physics Condensed Matter, 2004, 16, 8251-8266.	1.8	86
56	Charge injection in molecular wires grafted on metallic surfaces: electron-lattice interaction. European Physical Journal D, 2003, 24, 409-412.	1.3	3
57	Observational Indicators of Formation Excitation of H2. Astrophysics and Space Science, 2003, 288, 377-389.	1.4	19
58	Simulation of spin-resolved scanning tunneling microscopy: influence of the magnetization of surface and tip. Journal of Magnetism and Magnetic Materials, 2003, 267, 139-151.	2.3	13
59	Optically driven silicon-based quantum gates with potential for high-temperature operation. Journal of Physics Condensed Matter, 2003, 15, L447-L451.	1.8	125
60	Surface Coverage Effects on the Formation of Molecular Hydrogen on a Graphite Surface via an Eleyâ^'Rideal Mechanism. Journal of Physical Chemistry A, 2003, 107, 10862-10871.	2.5	20
61	Signature of a Chemical Bond in the Conductance between Two Metal Surfaces. Physical Review Letters, 2003, 91, 036803.	7.8	70
62	Soliton effects in dangling-bond wires on Si(001). Physical Review B, 2003, 68, .	3.2	12
63	Quantum computing in the solid state: the challenge of decoherence. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2003, 361, 1441-1450.	3.4	18
64	Diffusion of a polaron in dangling bond wires on Si(001). Journal of Physics Condensed Matter, 2002, 14, L749-L755.	1.8	6
65	Mechanisms for electron transport in atomic-scale one-dimensional wires: Soliton and polaron effects. Europhysics Letters, 2002, 57, 885-891.	2.0	17
66	Describing mixed spin-space entanglement of pure states of indistinguishable particles using an occupation-number basis. Physical Review A, 2002, 66, .	2.5	76
67	Tip effects in scanning tunneling microscopy of atomic-scale magnetic structures. Surface Science, 2002, 498, L65-L70.	1.9	11
68	Understanding electron flow in conducting polymer films: injection, mobility, recombination and mesostructure. Journal of Physics Condensed Matter, 2002, 14, 9877-9898.	1.8	36
69	Coherent electron injection and transport in molecular wires: inelastic tunneling and electron–phonon interactions. Chemical Physics, 2002, 281, 279-292.	1.9	21
70	Determining surface magnetization and local magnetic moments with atomic scale resolution. Surface Science, 2002, 515, L487-L492.	1.9	6
71	Tuning in on single molecular states: adsorption sites and STM images of maleic anhydride on Si(100). Chemical Physics Letters, 2002, 355, 347-354.	2.6	22
72	Electronic structure and STM images of self-assembled styrene lines on a Si(100) surface. Chemical Physics Letters, 2002, 365, 129-134.	2.6	34

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73	Time-Dependent Quantum Mechanical Calculations on the Formation of Molecular Hydrogen on a Graphite Surface via an Eleyâ^Rideal Mechanismâ€. Journal of Physical Chemistry A, 2001, 105, 2173-2182.	2.5	84
74	Adsorption sites and STM images of C2H2 on Si(100): a first-principles study. Surface Science, 2001, 475, 83-88.	1.9	38
75	Benzene on silicon: combining STM experiments with first principles studies. Surface Science, 2001, 482-485, 1181-1185.	1.9	23
76	Adsorption of benzene on Si(100)-(2×1): Adsorption energies and STM image analysis byab initiomethods. Physical Review B, 2001, 63, .	3.2	91
77	Does Luttinger liquid behaviour survive in an atomic wire on a surface?. Journal of Physics Condensed Matter, 2001, 13, 5035-5046.	1.8	10
78	Series of(n×2)Si-rich reconstructions of β-SiC(001):â€, A prospective atomic wire. Physical Review B, 2001, 63, .	3.2	16
79	Coherent electron-phonon coupling and polaronlike transport in molecular wires. Physical Review B, 2001, 63, .	3.2	113
80	Surface Relaxations, Current Enhancements, and Absolute Distances in High Resolution Scanning Tunneling Microscopy. Physical Review Letters, 2001, 87, 236104.	7.8	134
81	Formation of molecular hydrogen on a graphite surface via an Eley–Rideal mechanism. Chemical Physics Letters, 2000, 319, 303-308.	2.6	97
82	Modeling of the β-SiC(001) (3×2) surface reconstruction. Applied Surface Science, 2000, 162-163, 94-99.	6.1	5
83	Transmission through Peierls distorted one-dimensional atomic wires: quantum coherent electron–phonon coupling. Applied Surface Science, 2000, 162-163, 613-619.	6.1	7
84	Modeling thec(4×2)reconstruction ofβâ^'SiC(001). Physical Review B, 2000, 62, 6904-6907.	3.2	11
85	Small polaron formation in dangling-bond wires on the Si(001) surface. Physical Review B, 2000, 63, .	3.2	18
86	STM experiment and atomistic modelling hand in hand: individual molecules on semiconductor surfaces. Surface Science Reports, 1999, 33, 1-81.	7.2	71
87	Quantum Inelastic Conductance through Molecular Wires. Physical Review Letters, 1999, 83, 452-455.	7.8	134
88	Atom extraction from an MoS 2 surface with a scanning tunnelling microscope: an ab initio study. Applied Physics A: Materials Science and Processing, 1998, 66, S741-S744.	2.3	2
89	Dynamical effective potential for tunneling: an exact matrix method and a path-integral technique. Applied Physics A: Materials Science and Processing, 1998, 66, S919-S923.	2.3	7
90	Potential dependence of polaron and bipolaron densities in conducting polymers: theoretical description beyond the Nernst equations. Chemical Physics, 1998, 227, 219-241.	1.9	33

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91	A matrix method for treating the coupling between an electron and a surface plasmon: a dynamical image potential in model tunnelling junctions. Journal of Physics Condensed Matter, 1998, 10, 3697-3718.	1.8	12
92	Studies of implanted muons in organic radicals. Journal of Physics Condensed Matter, 1998, 10, 10701-10713.	1.8	4
93	Ab initiostudy of STM-induced vacancy formation on the surface. Journal of Physics Condensed Matter, 1998, 10, 4533-4551.	1.8	1
94	The influence of an electric field on the electronic structure of a surface containing defects: an embedding-potential approach. Journal of Physics Condensed Matter, 1997, 9, 1793-1811.	1.8	2
95	Anab initiostudy of muons in ethanal. Journal of Physics Condensed Matter, 1997, 9, 3241-3257.	1.8	6
96	Ab initiostudies of magnetism in the organic radicalp-NPNN. Journal of Physics Condensed Matter, 1997, 9, 3635-3645.	1.8	4
97	Nonperturbative evaluation of STM tunneling probabilities fromab initiocalculations. Physical Review B, 1997, 56, 12469-12481.	3.2	42
98	Influence of the tip-induced electric field on the STM contrast of chemisorbedC2H4on the Si(001) surface. Physical Review B, 1997, 55, 10081-10093.	3.2	47
99	Bifurcations and the transition to chaos in the resonant-tunneling diode. Physical Review B, 1997, 56, 3913-3921.	3.2	25
100	Electronic structure and scanning tunnelling microscope images of missing-atom defects on and surfaces. Journal of Physics Condensed Matter, 1997, 9, 3671-3686.	1.8	14
101	Hydrocarbon adsorption on Si(001): when does the Si dimer bond break?. Surface Science, 1997, 374, 298-305.	1.9	97
102	Tip-induced surface polarization: a new mechanism for contrast in the scanning tunnelling microscope. Surface Science, 1997, 380, L479-L484.	1.9	18
103	Theoretical studies of processes involving implanted muons. Current Opinion in Solid State and Materials Science, 1996, 1, 841-845.	11.5	2
104	Potential for a novel μSR experiment — the results of an ab initio study. Chemical Physics Letters, 1996, 259, 271-275.	2.6	7
105	Theoretical studies of implanted muons in organic magnets. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1996, 37, 247-250.	3.5	3
106	Path-integral simulations of zero-point effects for implanted muons in benzene. Chemical Physics Letters, 1995, 242, 1-6.	2.6	33
107	μSR studies of magnetism in the organic systems p-NPNN and 3-QNNN. Synthetic Metals, 1995, 71, 1823-1824.	3.9	14
108	Adsorption and scanning-tunneling-microscope imaging of benzene on graphite andMoS2. Physical Review Letters, 1993, 70, 3263-3266.	7.8	136

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109	Organic ferromagnetism in the nitronyl nitroxides p-NPNN and 3-QNNN: MUSR, EPR and a.c. susceptibility studies. Synthetic Metals, 1993, 61, 171-175.	3.9	33
110	Defect electronic states in beta -carotene and lower homologues. Journal of Physics Condensed Matter, 1993, 5, 7049-7062.	1.8	4
111	Adsorption and STM imaging of organic molecules from first principles. , 1993, , 185-197.		1
112	Magnetotransport and Fermi-surface topology of [bis(ethylenedithio)tetrathiafulvalene]2KHg(SCN)4. Physical Review B, 1992, 45, 13904-13912.	3.2	72
113	Theory of defects in conducting polymers. II. Application to polyacetylene. Journal of Physics Condensed Matter, 1991, 3, 3905-3920.	1.8	22
114	Title is missing!. Journal of Physics Condensed Matter, 1991, 3, 9823-9829.	1.8	9
115	Theory of defects in conducting polymers. I. Theoretical principles and simple applications. Journal of Physics Condensed Matter, 1991, 3, 3879-3903.	1.8	53
116	A modified form for the real-space embedding potential. Journal of Physics Condensed Matter, 1990, 2, 6079-6082.	1.8	9
117	Theory of the structure of the self-trapped exciton in quartz. Journal of Physics Condensed Matter, 1990, 2, 6707-6720.	1.8	33
118	Structure of the self-trapped exciton in quartz. Physical Review Letters, 1990, 64, 2667-2670.	7.8	86
119	Polarons and solitons. Journal of Physics Condensed Matter, 1989, 1, 5567-5593.	1.8	32
120	The embedding potential for an interacting system. Journal of Physics Condensed Matter, 1989, 1, 3883-3895.	1.8	2
121	Theoretical studies of the blue luminescence in α-quartz. Journal of the Chemical Society, Faraday Transactions 2, 1989, 85, 467-469.	1.1	4
122	Quantum oscillations and negative magnetoresistance in the organic metal β''(BEDT-TTF)2AuBr2. Physical Review Letters, 1988, 61, 2721-2724.	7.8	29
123	Methods of embedding for defect and surface problems. Journal of Physics C: Solid State Physics, 1988, 21, 3229-3249.	1.5	14
124	A comparison of techniques for embedding defect cluster calculations. Theoretica Chimica Acta, 1987, 72, 319-324.	0.8	9