Ben J Powell

List of Publications by Year
in descending order

113 papers	4,222 citations	147801 31 h-index	114465 63 g-index
121 all docs	121 docs citations	121 times ranked	4633 citing authors

#	Article	IF	Citations
1	Towards quantum chemistry on a quantum computer. Nature Chemistry, 2010, 2, 106-111.	13.6	568
2	Role of semiconductivity and ion transport in the electrical conduction of melanin. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 8943-8947.	7.1	305
3	Quantum frustration in organic Mott insulators: from spin liquids to unconventional superconductors. Reports on Progress in Physics, 2011, 74, 056501.	20.1	267
4	Towards structureâ€“propertyâ€“function relationships for eumelanin. Soft Matter, 2006, 2, 37-44.	2.7	263
5	Chemical and Structural Disorder in Eumelanins: A Possible Explanation for Broadband Absorbance. Biophysical Journal, 2006, 90, 743-752.	0.5	230
6	A unified explanation of the Kadowakiâ€“Woods ratio in strongly correlated metals. Nature Physics, 2009, 5, 422-425.	16.7	173
7	A first-principles density-functional calculation of the electronic and vibrational structure of the key melanin monomers. Journal of Chemical Physics, 2004, 120, 8608-8615.	3.0	147
8	Strong electronic correlations in superconducting organic charge transfer salts. Journal of Physics Condensed Matter, 2006, 18, R827-R866.	1.8	146
9	Theories of phosphorescence in organo-transition metal complexes â€“ From relativistic effects to simple models and design principles for organic light-emitting diodes. Coordination Chemistry Reviews, 2015, 295, 46-79.	18.8	93
10	Half-Filled Layered Organic Superconductors and the Resonating-Valence-Bond Theory of the Hubbard-Heisenberg Model. Physical Review Letters, 2005, 94, 047004.	7.8	92
11	Effect of Irradiation-Induced Disorder on the Conductivity and Critical Temperature of the Organic Superconductorî²â˜²(BEDTâ˜²TTF)2Cu(SCN)2. Physical Review Letters, 2006, 96, 177002.	7.8	86
12	Hydration-Controlled X-Band EPR Spectroscopy: A Tool for Unravelling the Complexities of the Solid-State Free Radical in Eumelanin. Journal of Physical Chemistry B, 2013, 117, 4965-4972.	2.6	84
13	On the origin of electrical conductivity in the bio-electronic material melanin. Applied Physics Letters, 2012, 100, .	3.3	76
14	Spinâ€“Orbit Coupling in Phosphorescent Iridium(III) Complexes. ChemPhysChem, 2011, 12, 2429-2438.	2.1	73
15	Dependence of the superconducting transition temperature of organic molecular crystals on intrinsically nonmagnetic disorder: A signature of either unconventional superconductivity or the atypical formation of magnetic moments. Physical Review B, 2004, 69, .	3.2	70
16	Ferromagnetism, paramagnetism, and a Curie-Weiss metal in an electron-doped Hubbard model on a triangular lattice. Physical Review B, 2006, 73, .	3.2	70
17	Calculation of solid state molecular ionisation energies and electron affinities for organic semiconductors. Organic Electronics, 2011, 12, 394-403.	2.6	69
18	Symmetry of the Superconducting Order Parameter in Frustrated Systems Determined by the Spatial Anisotropy of Spin Correlations. Physical Review Letters, 2007, 98, 027005.	7.8	53

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19	Convergent Proton-Transfer Photocycles Violate Mirror-Image Symmetry in a Key Melanin Monomer. Journal of the American Chemical Society, 2007, 129, 6672-6673.	13.7	51
20	Gaseous Adsorption in Melanins: Hydrophilic Biomacromolecules with High Electrical Conductivities. Langmuir, 2010, 26, 412-416.	3.5	50
21	Bond Fission and Non-Radiative Decay in Iridium(III) Complexes. Inorganic Chemistry, 2016, 55, 5266-5273.	4.0	49
22	Effects of Fluorination on Iridium(III) Complex Phosphorescence: Magnetic Circular Dichroism and Relativistic Time-Dependent Density Functional Theory. Inorganic Chemistry, 2012, 51, 2821-2831.	4.0	48
23	The gap equations for spin singlet and triplet ferromagnetic superconductors. Journal of Physics A, 2003, 36, 9289-9302.	1.6	44
24	Geometrical Frustration in the Spin Liquid<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msup><mml:mi>Î²</mml:mi><mml:mo>â€²</mml:mo></mml:msup><mml:mtext mathvariant="normal">â^’</mml:mtext><mml:msub><mml:mi>Me</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi>EtSb</mml stretchy="false">[</mml:mo><mml:mi>Pd</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mi>dmit</mml:mi><mml:msub><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 517 Td (stretchy="	7.8	42
25	Elucidating the Spatial Arrangement of Emitter Molecules in Organic Lightâ€Emitting Diode Films. Angewandte Chemie - International Edition, 2017, 56, 8402-8406.	13.8	40
26	Relativistic effects in a phosphorescent Ir(III) complex. Physical Review B, 2011, 83, .	3.2	39
27	Spin-State Ice in Elastically Frustrated Spin-Crossover Materials. Journal of the American Chemical Society, 2019, 141, 19790-19799.	13.7	39
28	Effective Coulomb interactions within BEDT-TTF dimers. Physical Review B, 2009, 80, .	3.2	37
29	Mechanomagnetics in Elastic Crystals: Insights from [Cu(acac)₂]. Angewandte Chemie - International Edition, 2019, 58, 15082-15088.	13.8	36
30	Structureâ€"property relationships and the mechanisms of multistep transitions in spin crossover materials and frameworks. Inorganic Chemistry Frontiers, 2020, 7, 4424-4437.	6.0	36
31	Toward the parametrization of the Hubbard model for salts of bis(ethylenedithio)tetrathiafulvalene: A density functional study of isolated molecules. Journal of Chemical Physics, 2009, 130, 104508.	3.0	34
32	Nonradiative Decay and Stability of <i>N</i>-Heterocyclic Carbene Iridium(III) Complexes. Inorganic Chemistry, 2018, 57, 8881-8889.	4.0	31
33	Models of organometallic complexes for optoelectronic applications. Journal of Materials Chemistry, 2010, 20, 10301.	6.7	29
34	In-plane superfluid density and microwave conductivity of the organic superconductorÎº-(BEDT-TTF)2Cu[N(CN)2]Br: Evidence ford-wave pairing and resilient quasiparticles. Physical Review B, 2013, 88, .	3.2	28
35	Spin-liquid phase due to competing classical orders in the semiclassical theory of the Heisenberg model with ring exchange on an anisotropic triangular lattice. Physical Review B, 2014, 89, .	3.2	28
36	5,6-Dihydroxyindole-2-carboxylic acid: a first principles density functional study. Chemical Physics Letters, 2005, 402, 111-115.	2.6	26

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37	Three-dimensional carbazole-based dendrimers: model structures for studying charge transport in organic semiconductor films. Polymer Chemistry, 2013, 4, 916-925.	3.9	22
38	Transition dipole strength of eumelanin. Physical Review E, 2007, 76, 021915.	2.1	21
39	Mixed order parameters, accidental nodes and broken time reversal symmetry in organic superconductors: a group theoretical analysis. Journal of Physics Condensed Matter, 2006, 18, L575-L584.	1.8	20
40	Spin-liquid phase in a spatially anisotropic frustrated antiferromagnet: A Schwinger boson mean-field approach. Physical Review B, 2014, 89, .	3.2	20
41	Spin-orbit coupling and strong electronic correlations in cyclic molecules. Physical Review B, 2017, 95, .	3.2	19
42	Spin fluctuations and the pseudogap in organic superconductors. Physical Review B, 2009, 80, .	3.2	18
43	Interplay of dipoles and spins in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>Î¹</mml:mi><mml:mo>â^'</mml:mo><mml:msub><mml:m , where <mml:math		

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55	Synthesis and properties of pyrrolo[3,2-b]pyrrole-1,4-diones (isoDPP) derivatives. Journal of Materials Chemistry C, 2014, 2, 4276.	5.5	13
56	Emergent particles and gauge fields in quantum matter. Contemporary Physics, 2020, 61, 96-131.	1.8	13
57	Pomeranchuk instability: Symmetry-breaking and experimental signatures. Physica B: Condensed Matter, 2008, 403, 1279-1281.	2.7	12
58	Sensitivity of the photophysical properties of organometallic complexes to small chemical changes. Journal of Chemical Physics, 2010, 133, 124314.	3.0	12
59	Interplay of frustration, magnetism, charge ordering, and covalency in the ionic Hubbard model for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Na</mml:mtext></mml:mrow><mml:mrow><mml:mn>0.5</mm Physical Review B, 2009, 79, .	3.2	11
60	Electronic correlations in organometallic complexes. Chemical Physics Letters, 2011, 508, 22-28.	2.6	11
61	Kinetics of charge transfer processes in organic solar cells: Implications for the design of acceptor molecules. Organic Electronics, 2012, 13, 2538-2545.	2.6	11
62	Low-energy effective theories of the two-thirds filled Hubbard model on the triangular necklace lattice. Physical Review B, 2014, 90, .	3.2	11
63	Conservation laws, radiative decay rates and excited state localization in organometallic complexes with strong spin-orbit coupling. Scientific Reports, 2015, 5, 10815.	3.3	11
64	Exact exchange and the density functional theory of metal-to-ligand charge-transfer in fac-Ir(ppy)3. Organic Electronics, 2016, 33, 110-115.	2.6	11
65	Quasi-one-dimensional spin-orbit-coupled correlated insulator in a multinuclear coordinated organometallic crystal. Physical Review B, 2016, 94, .	3.2	10
66	A thiocarbonyl-containing small molecule for optoelectronics. RSC Advances, 2017, 7, 10316-10322.	3.6	10
67	Mechanomagnetics in Elastic Crystals: Insights from [Cu(acac) 2]. Angewandte Chemie, 2019, 131, 15226-15232.	2.0	10
68	Frustration, ring exchange, and the absence of long-range order in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>EtMe</mml:mi><mml:mn>3</mml:mn></mm From first principles to many-body theory. Physical Review Materials, 2020, 4, .	2.4	10
69	A phenomenological model of the superconducting state of the Bechgaard salts. Journal of Physics Condensed Matter, 2008, 20, 345234.	1.8	9
70	Effects of anisotropy in spin molecular-orbital coupling on effective spin models of trinuclear organometallic complexes. Physical Review B, 2017, 96, .	3.2	9
71	Quantitative calculations of the non-radiative rate of phosphorescent Ir(<scp>iii</scp>) complexes. Physical Chemistry Chemical Physics, 2020, 22, 27348-27356.	2.8	9
72	Dual-supramolecular contacts induce extreme Hofmann framework distortion and multi-stepped spin-crossover. Dalton Transactions, 2021, 50, 1434-1442.	3.3	9

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73	Ionic Hubbard model on a triangular lattice forNa0.5CoO2,Rb0.5CoO2, andK0.5CoO2: Mean-field slave boson theory. Physical Review B, 2009, 80, .	3.2	8
74	Magnetic excitations of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi>Cu</mml:mi></mml:mrow><mml:mrow><m quantum spin chain in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Sr</mml:mi><mml:mn>3</mml:mn></mml:r Physical Review B, 2018, 97, .	3.2	8
75	Toward High-Temperature Light-Induced Spin-State Trapping in Spin-Crossover Materials: The Interplay of Collective and Molecular Effects. Journal of the American Chemical Society, 2022, 144, 9138-9148.	13.7	8
76	Competition between disorder and exchange splitting in superconducting ZrZn2. Journal of Physics Condensed Matter, 2003, 15, L235-L241.	1.8	7
77	Electronic and magnetic properties of the ionic Hubbard model on the striped triangular lattice at34filling. Physical Review B, 2009, 80, .	3.2	7
78	Superconductivity in metal-mixed ion-implanted polymer films. Applied Physics Letters, 2006, 89, 152503.	3.3	6
79	Vertex corrections and the Korringa ratio in strongly correlated electron materials. Journal of Physics Condensed Matter, 2009, 21, 195601.	1.8	6
80	Superconductivity suppression and peak resistivity enhancement for thin crystals of Îºâ€(BEDTâ€TTF)₂Cu(SCN)₂. Physica Status Solidi (B): Basic Research, 2012, 249, 979-984.	1.5	6
81	Quasi-one dimensional magnetic interactions in the three-dimensional hyper-honeycomb framework [(C₂H₅)₃NH]₂Cu₂(C₂O₄₃. Physical Chemistry Chemical Physics, 2021, 23, 5012-5019.	2.8	6
82	Multiple insulating states due to the interplay of strong correlations and lattice geometry in a single-orbital Hubbard model. Physical Review B, 2021, 103, .	3.2	6
83	Unconventional superconductivity near a flat band in organic and organometallic materials. Physical Review B, 2021, 103, .	3.2	6
84	Spin-0 Mott insulator to metal to spin-1 Mott insulator transition in the single-orbital Hubbard model on the decorated honeycomb lattice. Physical Review B, 2021, 104, .	3.2	6
85	Regulation of Multistep Spin Crossover Across Multiple Stimuli in a 2-D Framework Material. Inorganic Chemistry, 2022, 61, 6641-6649.	4.0	6
86	Charge transport properties of carbazole dendrimers in organic field-effect transistors. Proceedings of SPIE, 2011, , .	0.8	5
87	Breakdown of the universality of the Kadowaki-Woods Ratio in multi-band metals. Physical Review B, 2015, 92, .	3.2	5
88	Effect of n-propyl substituents on the emission properties of blue phosphorescent iridium(iii) complexes. Journal of Chemical Physics, 2017, 146, 174305.	3.0	5
89	Multi-Redox Responsive Behavior in a Mixed-Valence Semiconducting Framework Based on Bis-[1,2,5]-thiadiazolo-tetracyanoquinodimethane. Journal of the American Chemical Society, 0, , .	13.7	5
90	Umklapp scattering in unconventional superconductors: Microwave conductivity shows that Îºâ~'(BEDTâ~'TTF)2Cu[N(CN)2]Br is a dxy superconductor. Physical Review B, 2019, 100, .	3.2	4

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91	Hierarchical Spinâ€Crossover Cooperativity in Hybrid 1D Chains of Fe^{II}â€1,2,4â€Triazole Trimers Linked by [Au(CN)₂]^{â^'} Bridges. Chemistry - A European Journal, 2021, 27, 5136-5141.	3.3	4
92	Multiple Coulomb phases with temperature-tunable ice rules in pyrochlore spin-crossover materials. Physical Review B, 2021, 104, .	3.2	4
93	Tight-Binding Approach to Pyrazine-Mediated Superexchange in Copperâ€“Pyrazine Antiferromagnets. Inorganic Chemistry, 2021, 60, 11907-11914.	4.0	4
94	Broadband Photon-harvesting Biomolecules for Photovoltaics. , 2006, , 35-65.		3
95	Competition between superconductivity and weak localization in metal-mixed ion-implanted polymers. Physical Review B, 2010, 81, .	3.2	3
96	Nuclear magnetic resonance in low-symmetry superconductors. Physical Review B, 2018, 97, .	3.2	3
97	The expanding materials multiverse. Science, 2018, 360, 1073-1074.	12.6	3
98	Fate of the Hebel-Slichter peak in superconductors with strong antiferromagnetic fluctuations. Physical Review Research, 2021, 3, .	3.6	3
99	Spin-Crossover 2-D Hofmann Frameworks Incorporating an Amide-Functionalized Ligand: N-(pyridin-4-yl)benzamide. Chemistry, 2021, 3, 360-372.	2.2	3
100	Spin-state smectics in spin crossover materials. Journal of Applied Physics, 2021, 129, .	2.5	3
101	The origin of the difference in the superconducting critical temperatures of the Î²Hand Î²Lphases of (BEDT-TTF)2I3. European Physical Journal Special Topics, 2004, 114, 363-365.	0.2	3
102	Preparation of metal mixed plastic superconductors: Electrical properties of tin-antimony thin films on plastic substrates. Journal of Applied Physics, 2009, 105, 093909.	2.5	2
103	Spin molecular-orbit coupling and magnetic properties of the decorated honeycomb layers of Mo3S7(dmit)3 crystals. AIP Advances, 2018, 8, .	1.3	2
104	xâ^'[Pd(dmit)2]2 as a quasi-one-dimensional scalene Heisenberg model. Physical Review Materials, 2021, 5, .	2.4	2
105	First-principle density-functional calculation of the Raman spectra of BEDT-TTF. European Physical Journal Special Topics, 2004, 114, 293-295.	0.2	1
106	Elucidating the Spatial Arrangement of Emitter Molecules in Organic Lightâ€Emitting Diode Films. Angewandte Chemie, 2017, 129, 8522-8526.	2.0	1
107	Balance and frustration in strongly correlated itinerant electron systems: An extension of Nagaoka's theorem. Physical Review B, 2017, 96, .	3.2	1
108	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>C</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:m symmetry breaking metal-insulator transitions in a flat band in the half-filled Hubbard model on the decorated honeycomb lattice. Physical Review B, 2022, 105, .	3.2	1

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109	Co-existence of five- and six-coordinate iron(<scp>ii</scp>) species captured in a geometrically strained spin-crossover Hofmann framework. Dalton Transactions, 2022, 51, 9596-9600.	3.3	1
110	A Tunable Metalâ€“Organic Resistance Thermometer. ChemPhysChem, 2011, 12, 116-121.	2.1	0
111	Equivalence of Electron-Vibration Interaction and Charge-Induced Force Variations: A New O(1) Approach to an Old Problem. Crystals, 2012, 2, 236-247.	2.2	0
112	Publisher's Note: Low-energy effective theories of the two-thirds filled Hubbard model on the triangular necklace lattice [Phys. Rev. B 90 , 035120 (2014)]. Physical Review B, 2020, 101, .	3.2	0
113	The Behaviour of a Triplet Superconductor in a Spin Only Magnetic Field. Lecture Notes in Physics, 2002, , 46-59.	0.7	0