

# Roser Valenti

## List of Publications by Year in descending order

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187  
papers

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citations

71102

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188  
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188  
docs citations

188  
times ranked

5715  
citing authors

#	ARTICLE	IF	CITATIONS
1	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	1.8	79
2	Phase diagram of a distorted kagome antiferromagnet and application to Y-kapellasite. Npj Computational Materials, 2022, 8, .	8.7	17
3	Role of disorder in electronic and magnetic properties of $\text{OAg}_3\text{O}_6$ . Physical Review B, 2022, 105, .	3.2	3
4	Magnetoelastic coupling anisotropy in the Kitaev material $\text{RuCl}_2$ . Physical Review B, 2022, 105, .	3.2	3
5	Statistical learning of engineered topological phases in the kagome superlattice of AV <sub>3</sub> Sb <sub>5</sub> . Npj Computational Materials, 2022, 8, .	8.7	6
6	Ultrasharp Lateral p-n Junctions in Modulation-Doped Graphene. Nano Letters, 2022, 22, 4124-4130.	9.1	12
7	Engineering topological phases guided by statistical and machine learning methods. Physical Review Research, 2021, 3, .	3.6	6
8	Anisotropic superconductivity in the spin-vortex antiferromagnetic superconductor $\text{CaK}_2\text{Mo}_2\text{O}_{10}$ . Physical Review B, 2021, 103, .	3.2	3
9	Angle-dependent thermodynamics of $\text{RuCl}_2$ . Physical Review B, 2021, 103, .	3.2	3
10	Containment efficiency and control strategies for the corona pandemic costs. Scientific Reports, 2021, 11, 6848.	3.3	25
11	Anomalous Quantum Oscillations in a Heterostructure of Graphene on a Proximate Quantum Spin Liquid. Physical Review Letters, 2021, 126, 097201.	7.8	18
12	Band-Order Anomaly at the $\text{Al}_2\text{O}_3/\text{SrTiO}_3$ Interface Drives the Electron-Mobility Boost. ACS Nano, 2021, 15, 4347-4356.	14.6	18
13	Predicting the cumulative medical load of COVID-19 outbreaks after the peak in daily fatalities. PLoS ONE, 2021, 16, e0247272.	2.5	4
14	Magnetoelastic coupling and effects of uniaxial strain in $\text{RuCl}_3$ from first principles. Physical Review B, 2021, 103, .	3.2	25
15	Electronic structure and coexistence of superconductivity with magnetism in $\text{Rb}_4\text{EuFe}_4\text{As}_4$ . Physical Review B, 2021, 103, .	3.2	17
16	Magnetization Process of Atacamite: A Case of Weakly Coupled $\text{S}_2$ Sawtooth Chains. Physical Review Letters, 2021, 126, 207201.	7.8	16
17	Modified Curie-Weiss law for $\text{S}_2$ magnets. Physical Review B, 2021, 103, .	3.2	3
18	Effects of spin-phonon coupling in frustrated Heisenberg models. Physical Review B, 2021, 104, .	3.2	4

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19	Elementary band representations for the single-particle Green's function of interacting topological insulators. <i>Physical Review B</i> , 2021, 104, .	3.2	7
20	Prediction of double-Weyl points in the iron-based superconductor $\text{CaKFe}_4\text{As}_5$ . <i>Physical Review B</i> , 2021, 104, .	3.2	5
21	Pseudoelasticity of $\text{SrNi}_2\text{P}_2$ Micropillar via Double Lattice Collapse and Expansion. <i>Nano Letters</i> , 2021, 21, 7913-7920.	9.1	2
22	Orbital occupancy and hybridization in strained $\text{SrVO}_3$ epitaxial films. <i>Physical Review Materials</i> , 2021, 5, .	2.4	7
23	Spin Vortex Crystal Order in Organic Triangular Lattice Compound. <i>Physical Review Letters</i> , 2021, 127, 147204.	7.8	3
24	Construction of heterolayer intermetallic crystals: Case studies of the 1144-phase TM-phosphides $\text{AB}(\text{TM})_4$ . <i>Physical Review B</i> , 2021, 104, .	2.4	3
25	Two-Particle Self-Consistent Method for the Multi-Orbital Hubbard Model. <i>Annalen Der Physik</i> , 2021, 533, 2000399.	2.4	9
26	Pressure-induced ferromagnetism in the topological semimetal $\text{EuCd}_2\text{As}_2$ . <i>Physical Review B</i> , 2021, 104, .	3.2	7
27	Towards a topological quantum chemistry description of correlated systems: The case of the Hubbard diamond chain. <i>Physical Review B</i> , 2021, 104, .	3.2	7
28	Semimetallic square-octagon two-dimensional polymer with high mobility. <i>Physical Review B</i> , 2021, 104, .	3.2	3
29	Variational wave functions for the spin-Peierls transition in the Su-Schrieffer-Heeger model with quantum phonons. <i>Physical Review B</i> , 2020, 102, .	3.2	7
30	Thermodynamic Perspective on Field-Induced Behavior of $\text{RuCl}_2$ . <i>Physical Review Letters</i> , 2020, 125, 097203.	7.8	42
31	Deconfinement of Mott localized electrons into topological and spin-orbit-coupled Dirac fermions. <i>Npj Quantum Materials</i> , 2020, 5, .	5.2	13
32	Nonlocal correlations in iron pnictides and chalcogenides. <i>Physical Review B</i> , 2020, 102, .	3.2	21
33	Charge ordering and low-temperature lattice distortion in the $\text{BEDT-TTF}_2\text{CF}_3\text{CF}_2\text{SO}_3$ dimer Mott insulator. <i>Physical Review B</i> , 2020, 101, .	3.2	1
34	Alleviating the sign problem in quantum Monte Carlo simulations of spin-orbit-coupled multiorbital Hubbard models. <i>Physical Review B</i> , 2020, 101, .	3.2	13
35	High-field quantum disordered state in $\text{RuCl}_2$ : Spin flips, bound states, and multiparticle continuum. <i>Physical Review B</i> , 2020, 101, .	3.2	13
36	Lattice dynamics in the spin-1/2 frustrated kagome compound herbertsmithite. <i>Physical Review B</i> , 2020, 101, .	3.2	13





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73	Synthesis successes. Nature Chemistry, 2017, 9, 608-609.	13.6	4
74	Breakdown of magnons in a strongly spin-orbital coupled magnet. Nature Communications, 2017, 8, 1152.	12.8	173
75	Magnetic fluctuations and superconducting properties of $\text{CaKFeAs}_4$ studied by NMR. Physical Review B, 2017, 96, .	3.2	40
76	Pressure-induced half-collapsed-tetragonal phase in $\text{CaKFeAs}_4$ . Physical Review B, 2017, 96, .	3.2	40
77	Models and materials for generalized Kitaev magnetism. Journal of Physics Condensed Matter, 2017, 29, 493002.	1.8	384
78	Influence of oxygen vacancies on two-dimensional electron systems at SrTiO <sub>3</sub> -based interfaces and surfaces. European Physical Journal: Special Topics, 2017, 226, 2457-2475.	2.6	18
79	Microscopic origin of the mobility enhancement at a spinel/perovskite oxide heterointerface revealed by photoemission spectroscopy. Physical Review B, 2017, 96, .	3.2	32
80	Combined experimental and theoretical studies of pressure effects in La <sub>2</sub> Sb. Physica Status Solidi (B): Basic Research, 2017, 254, 1600168.	1.5	2
81	<i>Ab initio</i> perspective on structural and electronic properties of iron-based superconductors. Physica Status Solidi (B): Basic Research, 2017, 254, 1600164.	1.5	16
82	Nature of optical excitations in the frustrated kagome compound herbertsmithite. Physical Review B, 2017, 96, .	3.2	16
83	Charge orders in organic charge-transfer salts. New Journal of Physics, 2017, 19, 103033.	2.9	14
84	Electronic excitations in $\text{Fe}_3\text{S}_4$ . Physical Review B, 2017, 95, .	3.2	16
85	Signatures of a gearwheel quantum spin liquid in a spin-1/2 pyrochlore molybdate Heisenberg antiferromagnet. Physical Review Materials, 2017, 1, .	3.2	16
86	Reduction of magnetic interlayer coupling in barlowite through isoelectronic substitution. Physical Review B, 2016, 94, .	3.2	30
87	Hubbard band versus oxygen vacancy states in the correlated electron metal $\text{SrVO}_3$ . Physical Review B, 2016, 94, .	3.2	40
88	Prospect of quantum anomalous Hall and quantum spin Hall effect in doped kagome lattice Mott insulators. Scientific Reports, 2016, 6, 25988.	3.3	28
89	Electron dichotomy on the surface augmented by many-body effects. Physical Review B, 2016, 93, .	3.2	20
90	Spontaneous symmetry breaking in correlated wave functions. Physical Review B, 2016, 93, .	3.2	8

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91	Challenges in design of Kitaev materials: Magnetic interactions from competing energy scales. Physical Review B, 2016, 93, .	3.2	368
92	Hydrostatic pressure response of an oxide-based two-dimensional electron system. Physical Review B, 2016, 93, .	3.2	11
93	Unconventional magnetism on a honeycomb lattice in $\text{Sr}_2\text{VO}_4$ by muon spin rotation. Physical Review B, 2016, 94, .	3.2	2
94	Magnetism, Spin Texture, and In-Gap States: Atomic Specialization at the Surface of Oxygen-Deficient $\text{SrTiO}_3$ . Physical Review Letters, 2016, 116, 157203.	7.8	55
95	Evidence for Eight-Node Mixed-Symmetry Superconductivity in a Correlated Organic Metal. Physical Review Letters, 2016, 116, 237001.	7.8	33
96	Emergent lattices with geometrical frustration in doped extended Hubbard models. Physical Review B, 2016, 94, .	3.2	7
97	Near-degeneracy of extended $s$ - $d$ bands in $\text{Sr}_2\text{VO}_4$ . Physical Review B, 2016, 94, .	3.2	34
98	Role of vertex corrections in the matrix formulation of the random phase approximation for the multiorbital Hubbard model. Physical Review B, 2016, 94, .	3.2	16
99	Pressure-Induced Conductivity in a Neutral Nonplanar Spin-Localized Radical. Journal of the American Chemical Society, 2016, 138, 11517-11525.	13.7	38
100	Origin of the superconducting state in the collapsed tetragonal phase of $\text{KFe}_2\text{As}_2$ . Physical Review B, 2015, 91, .	3.2	26
101	Analysis of the optical conductivity for $\text{AFe}_2\text{As}_2$ from first principles. Physical Review B, 2015, 91, .	3.2	29
102	Role of layer packing for the electronic properties of the organic superconductor $\text{AFe}_2\text{As}_2$ .		



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109	Localized versus itinerant states created by multiple oxygen vacancies in SrTiO <sub>3</sub> . New Journal of Physics, 2015, 17, 023034.	2.9	47
110	Effect of magnetic frustration on nematicity and superconductivity in iron chalcogenides. Nature Physics, 2015, 11, 953-958.	16.7	255
111	Charge transfer tuning by chemical substitution and uniaxial pressure in the organic complex tetramethoxypyrene $\pi$ -tetracyanoquinodimethane. Physical Chemistry Chemical Physics, 2015, 17, 4118-4126.	2.8	17
112	Electronic structure and de Haas-van Alphen frequencies in KFe <sub>2</sub> As <sub>2</sub> within LDA+DMFT. New Journal of Physics, 2014, 16, 083025.	2.9	17
113	Addendum: Orbital selective phase transition. Modern Physics Letters B, 2014, 28, 1491001.	1.9	0
114	Effect of isoelectronic doping on the honeycomb-lattice iridate $\text{IrO}_3$ . Physical Review B, 2014, 89, .	3.2	42
115	Dynamics of tungsten hexacarbonyl, dicobalt octacarbonyl, and their fragments adsorbed on silica surfaces. Journal of Chemical Physics, 2014, 140, 184706.	3.0	6
116	Valence bond liquid phase in the honeycomb lattice material $\text{LiRuO}_3$ . Physical Review B, 2014, 89, .	3.2	92
117	Correlation effects in the tetragonal and collapsed-tetragonal phase of $\text{LiCu}_2\text{O}(\text{CN})$ . Physical Review B, 2014, 89, .	3.2	27
118	Correlation effects in the tetragonal and collapsed-tetragonal phase of $\text{CaFeAs}_2$ . Physical Review B, 2014, 90, .	3.2	13
119	Theoretical prediction of a strongly correlated Dirac metal. Nature Communications, 2014, 5, 4261.	12.8	167
120	Giant pressure-induced volume collapse in the pyrite mineral MnS <sub>2</sub> . Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 5106-5110.	7.1	37
121	One-dimensional spin liquid, collinear, and spiral phases from uncoupled chains to the triangular lattice. Physical Review B, 2014, 89, .	3.2	29
122	Ab initio analysis of the tight-binding parameters and magnetic interactions in Na $\text{IrO}_3$ . Physical Review B, 2013, 88, .	3.2	164
123	Absence of Metallicity in K-doped Picene: Importance of Electronic Correlations. Physical Review Letters, 2013, 110, 216403.	7.8	53
124	First-principles determination of Heisenberg Hamiltonian parameters for the spin-12 kagome antiferromagnet $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$ . Physical Review B, 2013, 88, .	3.2	81
125	Mott correlated states in the underdoped two-dimensional Hubbard model: Variational Monte Carlo versus a dynamical cluster approximation. Physical Review B, 2013, 87, .	3.2	20
126	Origin of the insulating state in honeycomb iridates and rhodates. Physical Review B, 2013, 88, .	3.2	57



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127	ORBITAL SELECTIVE PHASE TRANSITION. Modern Physics Letters B, 2013, 27, 1330015.	1.9	4
128	Simulation of electron transport during electron-beam-induced deposition of nanostructures. Beilstein Journal of Nanotechnology, 2013, 4, 781-792.	2.8	5
129	Momentum spectrometer for electron-electron coincidence studies on superconductors. Review of Scientific Instruments, 2012, 83, 103905.	1.3	11
130	<i>Ab initio</i> study of the two-dimensional metallic state at the surface of SrTiO <sub>3</sub> : Importance of oxygen vacancies. Physical Review B, 2012, 86, .	3.2	54
131	<i>Ab initio</i> study of the two-dimensional metallic state at the surface of SrTiO <sub>3</sub> : Importance of oxygen vacancies. Physical Review B, 2012, 86, .	3.2	54
132	Dynamical cluster approximation within an augmented plane wave framework: Spectral properties of SrVO <sub>3</sub> . Physical Review B, 2012, 85, .	3.2	26
133	Orbital-Resolved Partial Charge Transfer from the Methoxy Groups of Substituted Pyrenes in Complexes with Tetracyanoquinodimethane: A NEXAFS Study. Journal of the American Chemical Society, 2012, 134, 4694-4699.	13.7	19
134	Simulation of structural and electronic properties of amorphous tungsten oxycarbides. New Journal of Physics, 2012, 14, 113028.	2.9	5
135	LDA+DMFT study of the effects of correlation in LiFeAs. Physical Review B, 2012, 85, .	3.2	91
136	Fermi Surface Topology of LaFePO and LiFeP. Physical Review Letters, 2012, 109, 236403.	7.8	23
137	Spontaneous dissociation of Co <sub>2</sub> (CO) <sub>8</sub> and autocatalytic growth of Co on SiO <sub>2</sub> : A combined experimental and theoretical investigation. Beilstein Journal of Nanotechnology, 2012, 3, 546-555.	2.8	44
138	Thermally induced crystal-to-crystal transformations accompanied by changes in the magnetic properties of a Cu <sub>11</sub> -p-hydroquinonate polymer. CrystEngComm, 2011, 13, 391-395.	2.6	15
139	Multistep Approach to Microscopic Models for Frustrated Quantum Magnets: The Case of the Natural Mineral Azurite. Physical Review Letters, 2011, 106, 217201.	7.8	109
140	Importance of itinerancy and quantum fluctuations for the magnetism in ironpnictides. Journal of Physics and Chemistry of Solids, 2011, 72, 324-328.	4.0	6
141	First principles determination of the model parameters in. Physica B: Condensed Matter, 2010, 405, S224-S228.	2.7	0
142	Can the Mott Insulator TiOCl be Metallized by Doping? A First-Principles Study. Physical Review Letters, 2010, 104, 146402.	7.8	11
143	Pressure-driven phase transitions in TiOCl and the family (Ca, Sr, Ba)Fe <sub>2</sub> As <sub>2</sub> . Journal of Physics Condensed Matter, 2010, 22, 164208.	1.8	4
144	Itinerant nature of magnetism in iron pnictides: A first-principles study. Physical Review B, 2010, 81, .	3.2	34

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145	Proposed Orbital Ordering in $MnV_2O_4$ from First-Principles Calculations. <i>Physical Review Letters</i> , 2009, 102, 216405.	7.8	87
146	Similarities between structural distortions under pressure and chemical doping in superconducting $BaFe_2As_2$ . <i>Nature Materials</i> , 2009, 8, 471-475.	27.5	266
147	Revision of Model Parameters for $d^2$ -Type Charge Transfer Salts: An <i>Ab Initio</i> Study. <i>Physical Review Letters</i> , 2009, 103, 067004.	7.8	170
148	Microscopic model for transitions from Mott to spin-Peierls insulator in $TiOCl$ . <i>Physical Review B</i> , 2008, 78, .	3.2	20
149	Two Pressure-Induced Transitions in $TiOCl$ : Mott Insulator to Anisotropic Metal. <i>Physical Review Letters</i> , 2008, 101, 136406.	7.8	31
150	Cu-based metalorganic systems: an ab initio study of the electronic structure. <i>New Journal of Physics</i> , 2007, 9, 26-26.	2.9	2
151	Microscopic modeling of a spin crossover transition. <i>New Journal of Physics</i> , 2007, 9, 448-448.	2.9	22
152	Cluster dynamical mean-field calculations for $TiOCl$ . <i>New Journal of Physics</i> , 2007, 9, 380-380.	2.9	11
153	Orbital Order in $ZnV_2O_4$ . <i>Physical Review Letters</i> , 2007, 99, 126401.	7.8	89
154	Classical and ab initio preparation of reliable structures for polymeric coordination compounds. <i>Comptes Rendus Chimie</i> , 2007, 10, 82-88.	0.5	3
155	Modified 1,4-hydroquinone ligands bridging $Cu$ ions – Building blocks for a new class of quantum magnets. <i>Comptes Rendus Chimie</i> , 2007, 10, 109-115.	0.5	9
156	Field-induced phase transition in a metalorganic spin-dimer system – a potential model system to study Bose-Einstein condensation of magnons. <i>Journal of Magnetism and Magnetic Materials</i> , 2007, 310, 1319-1321.	2.3	5
157	Ferromagnetism in the Fe-substituted spinel semiconductor $ZnGa_2O_4$ . <i>Journal of Physics Condensed Matter</i> , 2005, 17, 7417-7431.	1.8	5
158	Electronic structure of the spin-1/2 quantum magnet $TiOCl$ . <i>Physical Review B</i> , 2005, 72, .	3.2	34
159	$Na_2V_3O_7$ : A Frustrated Nanotubular System with Spin-1/2 Diamond Ring Geometry. <i>Physical Review Letters</i> , 2005, 95, 107201.	7.8	25
160	Spin gap formation in the quantum spin systems $TiOX$ , $X = Cl$ and $Br$ . <i>New Journal of Physics</i> , 2005, 7, 74-74.	2.9	24
161	$TiOCl$ , an orbital-ordered system?. <i>Europhysics Letters</i> , 2004, 67, 63-69.	2.0	44
162	Comparative study between two quantum spin systems $KCuCl_3$ and $TiCuCl_3$ . <i>Europhysics Letters</i> , 2002, 60, 309-315.	2.0	14

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163	Evidence for an Unconventional Magnetic Instability in the Spin-Tetrahedra System $\text{Cu}_2\text{Te}_2\text{O}_5\text{Br}_2$ . <i>Physical Review Letters</i> , 2001, 87, 227201.	7.8	79
164	Modeling the Electronic Behavior of $\text{LiV}_2\text{O}_5$ : A Microscopic Study. <i>Physical Review Letters</i> , 2001, 86, 5381-5384.	7.8	41
165	Dzyaloshinskii-Moriya interaction in $\text{NaV}_2\text{O}_5$ : A microscopic study. <i>Physical Review B</i> , 2000, 62, 14164-14170.	3.2	6
166	Test of the frustrated spin-cluster model to describe the low-temperature physics of $\text{NaV}_2\text{O}_5$ . <i>Physical Review B</i> , 2000, 62, R14617-R14620.	3.2	9
167	Novel nonreciprocal acoustic effects in antiferromagnets. <i>Europhysics Letters</i> , 1999, 45, 242-248.	2.0	0
168	Magnon Splitting Induced by Charge Ordering in $\text{NaV}_2\text{O}_5$ . <i>Physical Review Letters</i> , 1999, 82, 976-979.	7.8	52
169	J1-J2 model revisited: Phenomenology of $\text{CuGeO}_3$ . <i>Physical Review B</i> , 1997, 55, 5944-5952.	3.2	13
170	Spin-Peierls vs Peierls distortions in a family of conjugated polymers. <i>Physical Review B</i> , 1997, 56, 1751-1761.	3.2	17
171	Many-body valence-bond theory. <i>International Journal of Quantum Chemistry</i> , 1997, 65, 421-438.	2.0	26
172	Theory of nonreciprocal optical effects in antiferromagnets: The case of $\text{Cr}_2\text{O}_3$ . <i>Physical Review B</i> , 1996, 54, 433-440.	3.2	32
173	Frustration-induced Raman scattering in $\text{CuGeO}_3$ . <i>Physical Review B</i> , 1996, 54, R9635-R9638.	3.2	50
174	Microscopic Model of Nonreciprocal Optical Effects in $\text{Cr}_2\text{O}_3$ . <i>Physical Review Letters</i> , 1995, 75, 2766-2769.	7.8	32
175	The Mott-Hubbard Transition on the $D = \infty$ Bethe Lattice. <i>Europhysics Letters</i> , 1994, 27, 299-304.	2.0	11
176	Spin-charge separation at small length scales in the two-dimensional t-J model. <i>Physical Review B</i> , 1994, 50, 11313-11317.	3.2	4
177	A self-consistent cluster study of the Emery model. <i>Annalen Der Physik</i> , 1994, 506, 460-466.	2.4	16
178	Cluster expansion for the self-energy: A simple many-body method for interpreting the photoemission spectra of correlated Fermi systems. <i>Physical Review B</i> , 1993, 48, 418-425.	3.2	94
179	Luttinger liquid instability of the 2D t-J model: A variational study. <i>Physical Review Letters</i> , 1992, 68, 2402-2405.	7.8	64
180	Rigorous bounds for ground-state properties of correlated Fermi systems. <i>Physical Review B</i> , 1991, 44, 13203-13212.	3.2	12

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181	Rigorous lower bounds on the ground-state energy of correlated Fermi systems. Physical Review B, 1991, 44, 3995-3998.	3.2	9
182	Lower bounds for the ground-state energies of the two-dimensional Hubbard and t-J models. Physical Review B, 1991, 43, 13743-13746.	3.2	14
183	Topological long-range order for resonating-valence-bond structures. Physical Review B, 1991, 43, 723-727.	3.2	22
184	Resonating-valence-bond theory for the square-planar lattice. Physical Review B, 1991, 43, 719-722.	3.2	9
185	Exact lower bounds to the ground-state energy of spin systems: The two-dimensional S=1/2 antiferromagnetic Heisenberg model. Physical Review B, 1990, 41, 9611-9613.	3.2	11
186	Covalent excitations of a polyphene polymer via a Herndon-Simpson model. Computational and Theoretical Chemistry, 1989, 185, 287-296.	1.5	4
187	Multi-Center Magnon Excitations Open the Entire Brillouin Zone to Terahertz Magnetometry of Quantum Magnets. Advanced Quantum Technologies, 0, , 2200023.	3.9	2