

Harald O Jeschke

List of Publications by Year in descending order

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all docs

178
docs citations

178
times ranked

6424
citing authors

#	ARTICLE	IF	CITATIONS
1	Phase diagram of a distorted kagome antiferromagnet and application to Y-kapellasite. Npj Computational Materials, 2022, 8, .	3.5	17
2	Charge-Ordering and Structural Transition in the New Organic Conductor $\hat{\Gamma}^{\epsilon 2}$ -(BEDT-TTF) ₂ CF ₃ CF ₂ SO ₃ . Journal of Physical Chemistry C, 2022, 126, 1890-1900.	1.5	1
3	Hole doping and chemical pressure effects on the strong coupling superconductor PdTe. Physical Chemistry Chemical Physics, 2021, 23, 13331-13337.	1.3	1
4	Magnetization Process of Atacamite: A Case of Weakly Coupled S_{12} Sawtooth Chains. Physical Review Letters, 2021, 126, 207201.	2.9	16
5	Superconductivity with High Upper Critical Field in the Cubic Centrosymmetric $\hat{\Gamma}$ -Carbide Nb ₄ Rh ₂ C ₁₆ . ACS Materials Au, 2021, 1, 55-61.	2.6	16
6	Field-tunable toroidal moment in a chiral-lattice magnet. Nature Communications, 2021, 12, 5339.	5.8	13
7	Spin Vortex Crystal Order in Organic Triangular Lattice Compound. Physical Review Letters, 2021, 127, 147204.	2.9	3
8	Magnetic Field Induced Quantum Spin Liquid in the Two Coupled Trillium Lattices of K_2		

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19	Unusual electronic state of Sn in AgSnSe_2 . Physical Review B, 2020, 101, .		
20	Charge ordering and low-temperature lattice distortion in the $\hat{\Gamma}_2^2\text{-(BEDT-TTF)}_2\text{CF}_3\text{CF}_2\text{SO}_3$ dimer Mott insulator. Physical Review B, 2020, 101, .	1.1	1
21	From kagome strip to kagome lattice: Realizations of frustrated $S=12$ antiferromagnets in Ti(III) fluorides. Physical Review B, 2019, 99, .	1.1	19
22	Rashba-like spin splitting along three momentum directions in trigonal layered PtBi ₂ . Nature Communications, 2019, 10, 4765.	5.8	42
23	Large resistivity reduction in mixed-valent CsAuBr_3 under pressure. Physical Review B, 2019, 100, .		
24	Two magnetization plateaus in the kagome fluoride $\text{Cs}_2\text{LiTi}_3\text{F}_{12}$. Physical Review B, 2019, 100, .	1.1	16
25	Successive phase transitions and magnetization plateau in the spin-1 triangular-lattice antiferromagnet BaMn_2As_2 . Physical Review B, 2019, 100, .		
26	Pressure-induced superconductivity in BaMn_2As_2 with $\mathbf{B} \parallel \mathbf{c}$. Physical Review B, 2019, 100, .		
27	Pressure-induced superconductivity in BaMn_2As_2 with $\mathbf{B} \parallel \mathbf{c}$. Physical Review B, 2019, 100, .		
28	Breathing chromium spinels: a showcase for a variety of pyrochlore Heisenberg Hamiltonians. Npj Quantum Materials, 2019, 4, .	1.8	42
29	Novel Fe-Based Superconductor LaFe_2P_2 in Comparison with Traditional Prictides. Physical Review Letters, 2019, 123, 267001.		
30	Quantum and Classical Phases of the Pyrochlore Heisenberg Model with Competing Interactions. Physical Review X, 2019, 9, .	2.8	52
31	Role of the Open-Shell Character on the Pressure-Induced Conductivity of an Organic Donor-Acceptor Radical Dyad. Chemistry - A European Journal, 2018, 24, 5500-5505.	1.7	14
32	Enhanced superconducting transition temperatures in the rocksalt-type superconductors $\text{In}_x\text{Mg}_{1-x}$. Physical Review B, 2018, 98, 020501.		

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37	Evidence for Electronically Driven Ferroelectricity in a Strongly Correlated Dimerized BEDT-TTF Molecular Conductor. <i>Physical Review Letters</i> , 2018, 120, 247601.	2.9	30
38	Origin of the pressure-dependent T_c valley in superconducting simple cubic phosphorus. <i>Physical Review Materials</i> , 2018, 2, .	1.0	7
39	Nontrivial Role of Interlayer Cation States in Iron-Based Superconductors. <i>Physical Review Letters</i> , 2017, 118, 017204.	2.9	13
40	J Freezing and Hund's Rules in Spin-Orbit-Coupled Multiorbital Hubbard Models. <i>Physical Review Letters</i> , 2017, 118, 086401.	2.9	40
41	Basic electronic properties of iron selenide under variation of structural parameters. <i>Physical Review B</i> , 2017, 96, .	1.1	13
42	Influence of oxygen vacancies on two-dimensional electron systems at SrTiO ₃ -based interfaces and surfaces. <i>European Physical Journal: Special Topics</i> , 2017, 226, 2457-2475.	1.2	18
43	From magnetic order to spin-liquid ground states on the $S=1$ triangular lattice. <i>Physical Review B</i> , 2017, 96, .	1.1	13
44	Microscopic origin of the mobility enhancement at a spinel/perovskite oxide heterointerface revealed by photoemission spectroscopy. <i>Physical Review B</i> , 2017, 96, .	1.1	32
45	Combined experimental and theoretical studies of pressure effects in La ₂ Sb. <i>Physica Status Solidi (B): Basic Research</i> , 2017, 254, 1600168.	0.7	2
46	<i>Ab initio</i> perspective on structural and electronic properties of iron-based superconductors. <i>Physica Status Solidi (B): Basic Research</i> , 2017, 254, 1600164.	0.7	16
47	Electronic excitations in FeI_3 . <i>Physical Review B</i> , 2017, 95, .	1.1	12
48	Signatures of a gearwheel quantum spin liquid in a spin- $\frac{1}{2}$ pyrochlore molybdate Heisenberg antiferromagnet. <i>Physical Review Materials</i> , 2017, 1, .	1.2	12
49	Reduction of magnetic interlayer coupling in barlowite through isoelectronic substitution. <i>Physical Review B</i> , 2016, 94, .	1.1	30
50	Microscopic origin of the charge transfer in single crystals based on thiophene derivatives: A combined NEXAFS and density functional theory approach. <i>Journal of Chemical Physics</i> , 2016, 145, 034702.	1.2	12
51	Hubbard band versus oxygen vacancy states in the correlated electron metal SrVO_3 . <i>Physical Review B</i> , 2016, 94, .	1.1	16
52	Prospect of quantum anomalous Hall and quantum spin Hall effect in doped kagome lattice Mott insulators. <i>Scientific Reports</i> , 2016, 6, 25988.	1.6	28
53	Electron dichotomy on the SrTiO_3 surface augmented by many-body effects. <i>Physical Review B</i> , 2016, 93, .	1.1	26
54	Stabilization of the tetragonal structure in BaO_6 . <i>Physical Review B</i> , 2016, 93, .	1.1	6

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55	Challenges in design of Kitaev materials: Magnetic interactions from competing energy scales. Physical Review B, 2016, 93, .	1.1	368
56	Competition between disorder and Coulomb interaction in a two-dimensional plaquette Hubbard model. Physical Review B, 2016, 93, .	1.1	12
57	Hydrostatic pressure response of an oxide-based two-dimensional electron system. Physical Review B, 2016, 93, .	1.1	11
58	<i>Ab initio</i> determination of spin Hamiltonians with anisotropic exchange interactions: The case of the pyrochlore ferromagnet $\text{Lu}_2\text{V}_2\text{O}_7$. Physical Review B, 2016, 94, .	1.1	14
59	Magnetism, Spin Texture, and In-Gap States: Atomic Specialization at the Surface of Oxygen-Deficient SrTiO_3 . Physical Review Letters, 2016, 116, 157203.	2.9	55
60	Evidence for Eight-Node Mixed-Symmetry Superconductivity in a Correlated Organic Metal. Physical Review Letters, 2016, 116, 237001.	2.9	33
61	Near-degeneracy of extended s - d bands in $\text{Lu}_2\text{V}_2\text{O}_7$. Physical Review B, 2016, 94, .	1.1	34
62	Pressure-Induced Conductivity in a Neutral Nonplanar Spin-Localized Radical. Journal of the American Chemical Society, 2016, 138, 11517-11525.	6.6	38
63	Origin of the superconducting state in the collapsed tetragonal phase of KFe_2As_2 . Physical Review B, 2015, 91, .	2.0	20
64	Analysis of the optical conductivity for A_2X_2 compounds from first principles. Physical Review B, 2015, 91, .	2.1	29
65	Role of layer packing for the electronic properties of the organic superconductor A_2X_2 .		

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73	Unified picture of the doping dependence of superconducting transition temperatures in alkali metal/ammonia intercalated FeSe. <i>Physical Review B</i> , 2015, 91, .	1.1	55
74	Localized versus itinerant states created by multiple oxygen vacancies in SrTiO ₃ . <i>New Journal of Physics</i> , 2015, 17, 023034.	1.2	47
75	Effect of magnetic frustration on nematicity and superconductivity in iron chalcogenides. <i>Nature Physics</i> , 2015, 11, 953-958.	6.5	255
76	Charge transfer tuning by chemical substitution and uniaxial pressure in the organic complex tetramethoxypyrene-tetracyanoquinodimethane. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 4118-4126.	1.3	17
77	Electronic structure and de Haas-van Alphen frequencies in KFe ₂ As ₂ within LDA+DMFT. <i>New Journal of Physics</i> , 2014, 16, 083025.	1.2	17
78	Addendum: Orbital selective phase transition. <i>Modern Physics Letters B</i> , 2014, 28, 1491001.	1.0	0
79	Field-induced magnetic transitions in $\langle \text{mml:math} \rangle$		

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91	Nonthermal phase transitions in semiconductors induced by a femtosecond extreme ultraviolet laser pulse. <i>New Journal of Physics</i> , 2013, 15, 015016.	1.2	76
92	Non-thermal phase transitions in semiconductors under femtosecond XUV irradiation. , 2013, , .		6
93	Finite temperature and pressure molecular dynamics for BaFe \times As \times . <i>Physical Review B</i> , 2013, 88, .	1.1	8
94	Photon energy dependence of graphitization threshold for diamond irradiated with an intense XUV FEL pulse. <i>Physical Review B</i> , 2013, 88, .	1.1	33
95	Semiclassical approximation solved by Monte Carlo integration as an efficient impurity solver for dynamical mean field theory and its cluster extensions. <i>Physical Review B</i> , 2013, 88, .	1.1	4
96	<i>Ab initio</i> analysis of the tight-binding parameters and magnetic interactions in Na \times IrO \times . <i>Physical Review B</i> , 2013, 88, .	1.1	164
97	<i>Ab initio</i> analysis of the tight-binding parameters and magnetic interactions in Na \times IrO \times and CaFe \times . <i>Physical Review B</i> , 2013, 88, .	1.1	26
98	Absence of Metallicity in K-doped Picene: Importance of Electronic Correlations. <i>Physical Review Letters</i> , 2013, 110, 216403.	2.9	53
99	Why MgFeGe is not a superconductor. <i>Physical Review B</i> , 2013, 87, .	1.1	8
100	Nonthermal graphitization of diamond induced by a femtosecond x-ray laser pulse. <i>Physical Review B</i> , 2013, 88, .	1.1	37
101	Electronic properties of Fabre charge-transfer salts under various temperature and pressure conditions. <i>Physical Review B</i> , 2013, 87, .	1.1	31
102	First-principles determination of Heisenberg Hamiltonian parameters for the spin-12kagome antiferromagnet ZnCu \times (OH) \times Cl \times . <i>Physical Review B</i> , 2013, 88, .	1.1	81
103	Importance of anisotropy in the spin-liquid candidate Me \times EtSb[Pd(dmit) \times] \times . <i>Physical Review B</i> , 2013, 88, .	1.1	17
104	Mott correlated states in the underdoped two-dimensional Hubbard model: Variational Monte Carlo versus a dynamical cluster approximation. <i>Physical Review B</i> , 2013, 87, .	1.1	20
105	Origin of the insulating state in honeycomb iridates and rhodates. <i>Physical Review B</i> , 2013, 88, .	1.1	57
106	ORBITAL SELECTIVE PHASE TRANSITION. <i>Modern Physics Letters B</i> , 2013, 27, 1330015.	1.0	4
107	Simulation of electron transport during electron-beam-induced deposition of nanostructures. <i>Beilstein Journal of Nanotechnology</i> , 2013, 4, 781-792.	1.5	5
108	Momentum spectrometer for electron-electron coincidence studies on superconductors. <i>Review of Scientific Instruments</i> , 2012, 83, 103905.	0.6	11

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109	versus hydrostatic pressure-induced phase transitions in CaFe_2As_2 and BaFe_2As_2	1.1	49
110	General mechanism for orbital selective phase transitions. Physical Review B, 2012, 85, .	1.1	19
111	<i>Ab initio</i> study of the two-dimensional metallic state at the surface of SrTiO_3 : Importance of oxygen vacancies. Physical Review B, 2012, 86, .	1.1	54
112	$\text{Na}_2\text{Co}_2\text{O}_7$: a Molecular Orbital Crystal. Physical Review Letters, 2012, 109, 197201.	1.1	15
113	Dynamical cluster approximation within an augmented plane wave framework: Spectral properties of SrVO_3 . Physical Review B, 2012, 85, .	1.1	26
114	Multiferroic $\text{FeTe}_2\text{O}_5\text{Br}$: Alternating spin chains with frustrated interchain interactions. Physical Review B, 2012, 86, .	1.1	20
115	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, 12555-12562.	6.6	19
116	Temperature dependence of structural and electronic properties of the spin-liquid candidate $\text{BEDT-TTF}-(\text{BEDT-TTF})_x\text{Cu}$	1.1	54
117	Absorption of an organometallic platinum complex on silica: an <i>ab initio</i> study. New Journal of Physics, 2012, 14, 073040.	1.2	23
118	Simulation of structural and electronic properties of amorphous tungsten oxycarbides. New Journal of Physics, 2012, 14, 113028.	1.2	5
119	LDA+DMFT study of the effects of correlation in LiFeAs . Physical Review B, 2012, 85, .	1.1	91
120	Fermi Surface Topology of LaFePO and LiFeP . Physical Review Letters, 2012, 109, 236403.	2.9	23
121	Spontaneous dissociation of $\text{Co}_2(\text{CO})_8$ and autocatalytic growth of Co on SiO_2 : A combined experimental and theoretical investigation. Beilstein Journal of Nanotechnology, 2012, 3, 546-555.	1.5	44
122	Thermally induced crystal-to-crystal transformations accompanied by changes in the magnetic properties of a $\text{Cu}_{11}\text{-p}$ -hydroquinonate polymer. CrystEngComm, 2011, 13, 391-395.	1.3	15
123	CuCl_2	1.1	36
124	Multistep Approach to Microscopic Models for Frustrated Quantum Magnets: The Case of the Natural Mineral Azurite. Physical Review Letters, 2011, 106, 217201.	2.9	109
125	Anisotropic two-orbital Hubbard model: Single-site versus cluster Dynamical Mean-Field Theory. Annalen Der Physik, 2011, 523, 689-697.	0.9	3
126	Importance of itinerancy and quantum fluctuations for the magnetism in ironpnictides. Journal of Physics and Chemistry of Solids, 2011, 72, 324-328.	1.9	6

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127	Orbital-selective phase transition induced by different magnetic states: A dynamical cluster approximation study. Physical Review B, 2011, 84, .	1.1	13
128	Interaction of $W(\text{CO})_6$ with SiO_2 surfaces: A density functional study. Physical Review B, 2011, 84, .	1.1	13
129	CuCl_2	1.1	27
130	First principles determination of the model parameters in. Physica B: Condensed Matter, 2010, 405, S224-S228.	1.3	0
131	Can the Mott Insulator TiOCl be Metallized by Doping? A First-Principles Study. Physical Review Letters, 2010, 104, 146402.	2.9	11
132	Local moments and symmetry breaking in metallic PrMnSbO . Physical Review B, 2010, 82, .	1.1	33
133	Dynamical Cluster Approximation Study of the Anisotropic Two-Orbital Hubbard Model. Physical Review Letters, 2010, 104, 026402.	2.9	21
134	Modulation of pairing interaction in $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_8+\delta$ by an O dopant: A density functional theory study. Physical Review B, 2010, 82, .	1.1	7
135	Pressure-driven phase transitions in TiOCl and the family $(\text{Ca}, \text{Sr}, \text{Ba})\text{Fe}_2\text{As}_2$. Journal of Physics Condensed Matter, 2010, 22, 164208.	0.7	4
136	Itinerant nature of magnetism in iron pnictides: A first-principles study. Physical Review B, 2010, 81, .	1.1	34
137	Orbital character variation of the Fermi surface and doping dependent changes of the dimensionality in BaFe_2As_2 . Physical Review B, 2010, 81, .	1.1	55
138	Possible origin of the reduced ordered magnetic moment in iron pnictides: A dynamical mean-field theory study. Physical Review B, 2010, 81, .	1.1	26
139	Analysis of spin-density wave conductivity spectra of iron pnictides in the framework of density functional theory. Physical Review B, 2010, 82, .	1.1	26
140	Electronic structure studies of BaFe_2As_2 by angle-resolved photoemission spectroscopy. Physical Review B, 2009, 79, .	1.1	75
141	Microscopic origin of pressure-induced phase transitions in the iron pnictide superconductors AFe_2As_2 . Physical Review B, 2009, 80, .	1.1	58
142	Molecular dynamics simulations of laser-induced damage of nanostructures and solids. Applied Physics A: Materials Science and Processing, 2009, 96, 33-42.	1.1	24
143	Similarities between structural distortions under pressure and chemical doping in superconducting BaFe_2As_2 . Nature Materials, 2009, 8, 471-475.	13.3	266
144	Fast impurity solver based on equations of motion and decoupling. Physical Review B, 2009, 79, .	1.1	17

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145	Revision of Model Parameters for $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"> \langle \text{mml:mi} \rangle \hat{\rho} \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle$ -Type Charge Transfer Salts: An <i>Ab Initio</i> Study. Physical Review Letters, 2009, 103, 067004.	2.9	170
146	First principles perspective on the microscopic model for Cs_2CuCl_4 and Cs_2CuBr_4 . Journal of Physics: Conference Series, 2009, 145, 012038.	0.3	6
147	Microscopic model for transitions from Mott to spin-Peierls insulator in TiOCl. Physical Review B, 2008, 78, .	1.1	20
148	Two Pressure-Induced Transitions in TiOCl: Mott Insulator to Anisotropic Metal. Physical Review Letters, 2008, 101, 136406.	2.9	31
149	Cu-based metalorganic systems: an ab initio study of the electronic structure. New Journal of Physics, 2007, 9, 26-26.	1.2	2
150	Microscopic modeling of a spin crossover transition. New Journal of Physics, 2007, 9, 448-448.	1.2	22
151	Microscopic investigation of laser-induced structural changes in single-wall carbon nanotubes. Physical Review B, 2007, 75, .	1.1	15
152	Microscopic model for the frustrated Cu spin tetrahedron-based $\text{Cu}_4\text{Te}_5\text{O}_{12}\text{X}_4$ (X=Cl, Br) systems. Physical Review B, 2007, 75, .	1.1	6
153	Classical and ab initio preparation of reliable structures for polymeric coordination compounds. Comptes Rendus Chimie, 2007, 10, 82-88.	0.2	3
154	Comparative investigation of the coupled-tetrahedra quantum spin systems $\text{Cu}_2\text{Te}_2\text{O}_5\text{X}_2$, X=Cl, Br and $\text{Cu}_4\text{Te}_5\text{O}_{12}\text{Cl}_4$. Physica C: Superconductivity and Its Applications, 2007, 460-462, 462-463.	0.6	1
155	Laser manipulation of nanodiamonds. Computational Materials Science, 2006, 35, 179-182.	1.4	6
156	Breathing coherent phonons and caps fragmentation in carbon nanotubes following ultrafast laser pulses. Physical Review B, 2006, 74, .	1.1	32
157	Large-amplitude coherent phonons and inverse Stone-Wales transitions in graphitic systems with defects interacting with ultrashort laser pulses. Physical Review B, 2006, 74, .	1.1	15
158	Decoupling method for dynamical mean-field theory calculations. Physical Review B, 2005, 71, .	1.1	23
159	Femtosecond Laser Nanosurgery of Defects in Carbon Nanotubes. Nano Letters, 2005, 5, 1361-1365.	4.5	31
160	Laser-induced coherent phonons in graphite and carbon nanotubes: model and simulations. Applied Physics A: Materials Science and Processing, 2004, 79, 855-857.	1.1	15
161	Atomistic simulation of the laser induced damage in single wall carbon nanotubes: Diameter and chirality dependence. Applied Physics A: Materials Science and Processing, 2004, 79, 899-901.	1.1	5
162	Selective Cap Opening in Carbon Nanotubes Driven by Laser-Induced Coherent Phonons. Physical Review Letters, 2004, 92, 117401.	2.9	54

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163	Theoretical approach to the laser-induced melting of graphite under different pressure conditions. Applied Surface Science, 2003, 208-209, 61-70.	3.1	15
164	Properties of Liquid Silicon Observed by Time-Resolved X-Ray Absorption Spectroscopy. Physical Review Letters, 2003, 91, 157403.	2.9	83
165	Properties of liquid silicon and carbon studied by ultrafast time-resolved x-ray absorption spectroscopy. Springer Series in Chemical Physics, 2003, , 39-41.	0.2	0
166	Time-dependent energy absorption changes during ultrafast lattice deformation. Journal of Applied Physics, 2002, 91, 18.	1.1	39
167	Theoretical description of the ultrafast ablation of diamond and graphite: dependence of thresholds on pulse duration. Applied Surface Science, 2002, 197-198, 107-113.	3.1	36
168	Laser ablation thresholds of silicon for different pulse durations: theory and experiment. Applied Surface Science, 2002, 197-198, 839-844.	3.1	124
169	Nonthermal fragmentation of C60. Chemical Physics Letters, 2002, 352, 154-162.	1.2	22
170	Femtosecond laser-induced ablation of graphite. Springer Series in Chemical Physics, 2001, , 425-427.	0.2	15
171	Theory for the Ultrafast Ablation of Graphite Films. Physical Review Letters, 2001, 87, 015003.	2.9	170
172	Theory for the ultrafast dynamics of excited clusters: interplay between elementary excitations and atomic structure. Applied Physics B: Lasers and Optics, 2000, 71, 361-371.	1.1	6
173	Femtosecond laser-induced ablation of graphite. , 2000, , .		1
174	Theory for laser-induced ultrafast phase transitions in carbon. Applied Physics A: Materials Science and Processing, 1999, 69, S49-S53.	1.1	36
175	Microscopic analysis of the laser-induced femtosecond graphitization of diamond. Physical Review B, 1999, 60, R3701-R3704.	1.1	93
176	Ultrafast Structural Response and Nonlinear Fragmentation Dynamics of Small Clusters Induced by Optical Excitation. Springer Series in Cluster Physics, 1999, , 181-208.	0.3	0
177	Theory for the ultrafast structural response of optically excited small clusters: Time dependence of the ionization potential. Physical Review A, 1996, 54, R4601-R4604.	1.0	17
178	Analysis of the ultrafast dynamics of the silver trimer upon photodetachment. Journal of Physics B: Atomic, Molecular and Optical Physics, 1996, 29, L545-L549.	0.6	11