

Wei Cao

List of Publications by Year in descending order

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125
papers

2,876
citations

218677

26
h-index

214800

47
g-index

125
all docs

125
docs citations

125
times ranked

3982
citing authors

#	ARTICLE	IF	CITATIONS
1	Discerning phase-matrices for individual nitride inclusions within ultra-high-strength steel: experiment driven DFT investigation. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 1456-1461.	2.8	3
2	Exploring Mechanisms of Hydration and Carbonation of MgO and Mg(OH) ₂ in Reactive Magnesium Oxide-Based Cements. <i>Journal of Physical Chemistry C</i> , 2022, 126, 6196-6206.	3.1	18
3	Family of Two-Dimensional Transition Metal Dichlorides: Fundamental Properties, Structural Defects, and Environmental Stability. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 2165-2172.	4.6	19
4	Interlayer Registry Index of Layered Transition Metal Dichalcogenides. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3353-3359.	4.6	3
5	Unveiling Non-isothermal Crystallization of CaO-Al ₂ O ₃ -B ₂ O ₃ -Na ₂ O-Li ₂ O-SiO ₂ Glass via <i>In Situ</i> X-ray Scattering and Raman Spectroscopy. <i>Inorganic Chemistry</i> , 2022, 61, 7017-7025.	4.0	7
6	Nickel nanoparticle-activated MoS ₂ for efficient visible light photocatalytic hydrogen evolution. <i>Nanoscale</i> , 2022, 14, 8601-8610.	5.6	11
7	Quantitative prediction of yield strength of highly alloyed complex steel using high energy synchrotron X-ray diffractometry. <i>Journal of Materials Research and Technology</i> , 2022, , .	5.8	0
8	Recent understanding of solid-liquid friction in ionic liquids. <i>Green Chemical Engineering</i> , 2021, 2, 145-157.	6.3	25
9	Adsorption of CO ₂ on the 1%Fe (0001) surface: insights from density functional theory. <i>RSC Advances</i> , 2021, 11, 6825-6830.	3.6	0
10	Incorporation of Si atoms into CrCoNiFe high-entropy alloy: a DFT study. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 135703.	1.8	5
11	First-Principles Prediction of Two-Dimensional B ₃ C ₂ P ₃ and B ₂ C ₄ P ₂ : Structural Stability, Fundamental Properties, and Renewable Energy Applications. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3436-3442.	4.6	34
12	Vacancy-Induced Niobate Perovskite-Tungsten Bronze Composite for Synergetic Tuning of Ferroelectricity and Band Gaps. <i>Journal of Physical Chemistry C</i> , 2021, 125, 8890-8898.	3.1	8
13	Interfacial ferroelectricity by van der Waals sliding. <i>Science</i> , 2021, 372, 1462-1466.	12.6	262
14	Fluorination to enhance superlubricity performance between self-assembled monolayer and graphite in water. <i>Journal of Colloid and Interface Science</i> , 2021, 596, 44-53.	9.4	15
15	Surface plasmon-driven photocatalytic activity of Ni@NiO/NiCO ₃ core-shell nanostructures. <i>RSC Advances</i> , 2021, 11, 2733-2743.	3.6	18
16	In-situ quantification and density functional theory elucidation of phase transformation in carbon steel during quenching and partitioning. <i>Acta Materialia</i> , 2021, 221, 117361.	7.9	12
17	Fabrication of FeNi hydroxides double-shell nanotube arrays with enhanced performance for oxygen evolution reaction. <i>Applied Catalysis B: Environmental</i> , 2020, 261, 118193.	20.2	99
18	Impacts of Stress Relief Treatments on Microstructure, Mechanical and Corrosion Properties of Metal Active-Gas Welding Joint of 2205 Duplex Stainless Steel. <i>Materials</i> , 2020, 13, 4272.	2.9	7

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19	Synergistic effect of Ni ²⁺ -Ag ⁺ -rutile TiO ₂ ternary nanocomposite for efficient visible-light-driven photocatalytic activity. RSC Advances, 2020, 10, 36930-36940.	3.6	6
20	Excellent Protein Immobilization and Stability on Heterogeneous TiO ₂ Hybrid Nanostructures: A Single Protein AFM Study. Langmuir, 2020, 36, 9323-9332.	3.5	9
21	Harnessing photo/electro-catalytic activity via nano-junctions in ternary nanocomposites for clean energy. Nanoscale, 2020, 12, 23461-23479.	5.6	18
22	Microstructural Evolution Induced Mechanical Property Enhancement in Cryogenically Rolled Ce-Modified SAF2507 Super Duplex Stainless Steel. Advanced Engineering Materials, 2020, 22, 2000516.	3.5	1
23	Impact of various dopant elements on the electronic structure of Cu ₂ ZnSnS ₄ (CZTS) thin films: a DFT study. CrystEngComm, 2020, 22, 5786-5791.	2.6	8
24	The interaction of two-dimensional $\hat{1}\pm$ - and $\hat{1}^2$ -phosphorus carbide with environmental molecules: a DFT study. Physical Chemistry Chemical Physics, 2020, 22, 11307-11313.	2.8	6
25	Antireflective design of Si-based photovoltaics via biomimicking structures on black butterfly scales. Solar Energy, 2020, 204, 738-747.	6.1	4
26	Vacuum brazing ZSCf composite ceramics to TC4 alloy with Ag-Cu filler. Journal of Materials Research and Technology, 2020, 9, 8627-8635.	5.8	12
27	Ab initio study of hydrogen sensing in Pd and Pt functionalized GaN [0001] nanowires. Applied Surface Science, 2020, 512, 146019.	6.1	7
28	The effect of surface wrinkles on the properties of water in graphene slit pores. Molecular Simulation, 2020, 46, 604-615.	2.0	3
29	[Ni(2,2'-bipy)3]Cl2 activated sepiolite clay with high photocatalytic and oil-water separation abilities. Journal of Industrial and Engineering Chemistry, 2019, 80, 33-42.	5.8	6
30	Ultrafast, Stable Ionic and Molecular Sieving through Functionalized Boron Nitride Membranes. ACS Applied Materials & Interfaces, 2019, 11, 30430-30436.	8.0	25
31	Generalized Scaling Law of Structural Superlubricity. Nano Letters, 2019, 19, 7735-7741.	9.1	42
32	Effect of brazing temperature on microstructure and mechanical properties of TiAl/ZrB ₂ joint brazed with CuTiZrNi filler. Journal of Manufacturing Processes, 2019, 46, 170-176.	5.9	16
33	Water Diffusion in Wiggling Graphene Membranes. Journal of Physical Chemistry Letters, 2019, 10, 7251-7258.	4.6	14
34	Controlled cold rolling effect on microstructure and mechanical properties of Ce-modified SAF 2507 super duplex stainless steel. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2019, 766, 138352.	5.6	27
35	Robust superlubricity by strain engineering. Nanoscale, 2019, 11, 2186-2193.	5.6	67
36	AFM Study of pH-Dependent Adhesion of Single Protein to TiO ₂ Surface. Advanced Materials Interfaces, 2019, 6, 1900411.	3.7	19

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37	Molecular Origin of Superlubricity between Graphene and a Highly Hydrophobic Surface in Water. Journal of Physical Chemistry Letters, 2019, 10, 2978-2984.	4.6	37
38	Direct Measurement of Adhesions of Liquids on Graphite. Journal of Physical Chemistry C, 2019, 123, 11671-11676.	3.1	7
39	Loading AgCl@Ag on phosphotungstic acid modified macrocyclic coordination compound: Z-scheme photocatalyst for persistent pollutant degradation and hydrogen evolution. Journal of Colloid and Interface Science, 2019, 547, 50-59.	9.4	23
40	Exfoliation of Two-Dimensional Materials: The Role of Entropy. Journal of Physical Chemistry Letters, 2019, 10, 981-986.	4.6	30
41	Determination of the small amount of proteins interacting with TiO ₂ nanotubes by AFM-measurement. Biomaterials, 2019, 192, 368-376.	11.4	19
42	Enhanced diffusion on oscillating surfaces through synchronization. Physical Review E, 2018, 97, 022141.	2.1	2
43	Metallic Contact between MoS ₂ and Ni via Au Nanogluue. Small, 2018, 14, e1704526.	10.0	32
44	Carbon nanostructure based mechano-nanofluidics. Journal of Micromechanics and Microengineering, 2018, 28, 033001.	2.6	8
45	Extrusion temperature impacts on biometallic Mg-2.0Zn-0.5Zr-3.0Gd (wt%) solid-solution alloy. Journal of Alloys and Compounds, 2018, 739, 468-480.	5.5	21
46	Comparison of Synthetic Routes for Large-scale Synthesis of Spherical BiVO ₄ with Photocatalytic and Superhydrophobic Properties. Chemistry Letters, 2018, 47, 148-151.	1.3	5
47	Cryorolling impacts on microstructure and mechanical properties of AISI 316 LN austenitic stainless steel. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2018, 709, 270-276.	5.6	42
48	Microstructures, Mechanical Properties, and Corrosion Behavior of As-Cast Mg-2.0Zn-0.5Zr-xGd (wt %) Biodegradable Alloys. Materials, 2018, 11, 1564.	2.9	19
49	Mechano-nanofluidics: water transport through CNTs by mechanical actuation. Microfluidics and Nanofluidics, 2018, 22, 1.	2.2	9
50	Synthesis of Ag-loaded Sb ₂ WO ₆ microsphere with enhanced photocatalytic ability for organic dyes degradations under different light irradiations. Journal of Molecular Liquids, 2018, 272, 27-36.	4.9	30
51	Effect of Rolling Temperature on Microstructure Evolution and Mechanical Properties of AISI316LN Austenitic Stainless Steel. Materials, 2018, 11, 1557.	2.9	23
52	Impacts of ionic liquid capping on the morphology and photocatalytic performance of SbPO ₄ crystals. CrystEngComm, 2018, 20, 4305-4312.	2.6	8
53	Water in Narrow Carbon Nanotubes: Roughness Promoted Diffusion Transition. Journal of Physical Chemistry C, 2018, 122, 19124-19132.	3.1	32
54	Brazing Ti-48Al-2Nb-2Cr Alloys with Cu-Based Amorphous Alloy Filler. Applied Sciences (Switzerland), 2018, 8, 920.	2.5	9

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55	Introducing Magnetism into 2D Nonmagnetic Inorganic Layered Crystals: A Brief Review from First-Principles Aspects. <i>Crystals</i> , 2018, 8, 24.	2.2	17
56	Tensile Creep Characterization and Prediction of Zr-Based Metallic Glass at High Temperatures. <i>Metals</i> , 2018, 8, 457.	2.3	7
57	Origin of hydration lubrication of zwitterions on graphene. <i>Nanoscale</i> , 2018, 10, 16887-16894.	5.6	36
58	Role of ultrafast dissociation in the fragmentation of chlorinated methanes. <i>Journal of Chemical Physics</i> , 2018, 148, 174301.	3.0	12
59	Hydrophilicity effect on CO ₂ /CH ₄ separation using carbon nanotube membranes: insights from molecular simulation. <i>Molecular Simulation</i> , 2017, 43, 502-509.	2.0	5
60	Strain enhanced lithium adsorption and diffusion on silicene. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 6563-6568.	2.8	30
61	Orienting spins in dually doped monolayer MoS ₂ : from one-sided to double-sided doping. <i>Chemical Communications</i> , 2017, 53, 5428-5431.	4.1	10
62	Transition Metal Adsorbed-Doped ZnO Monolayer: 2D Dilute Magnetic Semiconductor, Magnetic Mechanism, and Beyond 2D. <i>ACS Omega</i> , 2017, 2, 1192-1197.	3.5	22
63	One-pot hydrothermal synthesis of ZnC ₄ O ₄ concave microspheres with superhydrophobic and superoleophilic properties. <i>CrystEngComm</i> , 2017, 19, 528-536.	2.6	5
64	Brazing ZrB ₂ -SiC ceramics to Ti6Al4V alloy with TiCu-based amorphous filler. <i>Journal of Manufacturing Processes</i> , 2017, 30, 516-522.	5.9	41
65	Mass Production of Mesoporous MnCo ₂ O ₄ Spinels with Manganese(IV) and Cobalt(II)-Rich Surfaces for Superior Bifunctional Oxygen Electrocatalysis. <i>Angewandte Chemie</i> , 2017, 129, 15173-15177.	2.0	61
66	Evolution of lithium clusters to superatomic Li ₃₀ ⁺ . <i>Applied Physics Letters</i> , 2017, 111, .	3.3	3
67	SbVO ₄ nanoparticles synthesized via three facile one-pot methods: controllable morphologies and superhydrophobic coatings. <i>Dalton Transactions</i> , 2017, 46, 12988-12995.	3.3	5
68	Nanosecond laser coloration on stainless steel surface. <i>Scientific Reports</i> , 2017, 7, 7092.	3.3	21
69	Molecular Interactions of Protein with TiO ₂ by the AFM-Measured Adhesion Force. <i>Langmuir</i> , 2017, 33, 11626-11634.	3.5	25
70	Biogas upgrading using single-walled carbon nanotubes by molecular simulation. <i>Molecular Simulation</i> , 2017, 43, 1034-1044.	2.0	0
71	The effect of H ₂ O ₂ desorption on achieving improved selectivity for direct synthesis of H ₂ O ₂ over TiO ₂ (B)/anatase supported Pd catalyst. <i>Catalysis Communications</i> , 2017, 89, 69-72.	3.3	14
72	Phase and morphology controllable synthesis of superhydrophobic Sb ₂ O ₃ via a solvothermal method. <i>Journal of Alloys and Compounds</i> , 2017, 721, 149-156.	5.5	16

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73	The progress of quantitatively description of membrane process based on the mechanism of nanoconfined mass transfer. Chinese Science Bulletin, 2017, 62, 223-232.	0.7	1
74	Silicon 1s near edge X-ray absorption fine structure spectroscopy of functionalized silicon nanocrystals. Journal of Chemical Physics, 2016, 145, 154703.	3.0	2
75	Structural and dynamical properties of chlorinated hydrocarbons studied with resonant inelastic x-ray scattering. Journal of Chemical Physics, 2016, 144, 134309.	3.0	9
76	Ionic-liquid assisted ultrasonic synthesis of BiOCl with controllable morphology and enhanced visible light and sunlight photocatalytic activity. Journal of Molecular Catalysis A, 2016, 418-419, 132-137.	4.8	21
77	STRUCTURAL COLOR MODEL BASED ON SURFACE MORPHOLOGY OF MORPHO BUTTERFLY WING SCALE. Surface Review and Letters, 2016, 23, 1650046.	1.1	3
78	Formation of stable HCl resonant Auger decay in CH_3 . Physical Review A, 2016, 94, .	2.5	7
79	Shape-controlled hydrothermal synthesis of superhydrophobic and superoleophilic BaMnF ₄ micro/nanostructures. CrystEngComm, 2016, 18, 3585-3593.	2.6	10
80	Molecular Behavior of Water on Titanium Dioxide Nanotubes: A Molecular Dynamics Simulation Study. Journal of Chemical & Engineering Data, 2016, 61, 4131-4138.	1.9	12
81	Porous coordination polymer coatings fabricated from $\text{Cu}_3(\text{BTC})_2 \cdot 3\text{H}_2\text{O}$ with excellent superhydrophobic and superoleophilic properties. New Journal of Chemistry, 2016, 40, 10554-10559.	2.8	10
82	Molecular Simulation Study of the Adsorption and Diffusion of a Mixture of CO_2/CH_4 in Activated Carbon: Effect of Textural Properties and Surface Chemistry. Journal of Chemical & Engineering Data, 2016, 61, 4139-4147.	1.9	40
83	Diffusion of CO_2/CH_4 confined in narrow carbon nanotube bundles. Molecular Physics, 2016, 114, 2530-2540.	1.7	15
84	Separation of valence states in thin films with mixed V ₂ O ₅ and V ₇ O ₁₆ phases. Journal of Electron Spectroscopy and Related Phenomena, 2016, 211, 47-54.	1.7	7
85	First-principles study of monolayer MoS ₂ with deficient and excessive Mo and S ($n = \hat{a}^3 \hat{a}^3$) clusters on 5 Å–5 supercells. Computational Materials Science, 2016, 121, 124-130.	3.0	11
86	Controlled synthesis of hierarchical flower-like Sb ₂ WO ₆ microspheres: Photocatalytic and superhydrophobic property. Journal of Industrial and Engineering Chemistry, 2016, 39, 93-100.	5.8	34
87	Preparation and first-principles study for electronic structures of BiOI/BiOCl composites with highly improved photocatalytic and adsorption performances. Journal of Molecular Catalysis A, 2016, 423, 1-11.	4.8	52
88	Confined molecular motion across liquid/liquid interfaces in a triphasic reaction towards free-standing conductive polymer tube arrays. Journal of Materials Chemistry A, 2016, 4, 6290-6294.	10.3	7
89	Vacuum ultraviolet excitation luminescence spectroscopy of few-layered MoS ₂ . Journal of Physics Condensed Matter, 2016, 28, 015301.	1.8	13
90	Adsorption of binary CO_2/CH_4 mixtures using carbon nanotubes: Effects of confinement and surface functionalization. Separation Science and Technology, 2016, 51, 1079-1092.	2.5	4

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91	A computational study of antireflection structures bio-mimicked from leaf surface morphologies. <i>Solar Energy</i> , 2016, 131, 131-137.	6.1	22
92	Replication of Leaf Surface Structures for Light Harvesting. <i>Scientific Reports</i> , 2015, 5, 14281.	3.3	33
93	The pH-controlled morphology transition of BiVO ₄ photocatalysts from microparticles to hollow microspheres. <i>Materials Letters</i> , 2015, 145, 52-55.	2.6	41
94	X-RAY PHOTOEMISSION ELECTRON MICROSCOPE DETERMINATION OF ORIGINS OF ROOM TEMPERATURE FERROMAGNETISM AND PHOTOLUMINESCENCE IN HIGH-Co-CONTENT Zn _{1-x} O FILMS. <i>Surface Review and Letters</i> , 2014, 21, 1450058.	1.1	7
95	Breakdown of ionic character of molecular alkali bromides in inner-valence photoionization. <i>Journal of Chemical Physics</i> , 2014, 140, 204321.	3.0	1
96	Adsorption of N-Butane/I-Butane in Zeolites: Simulation and Theory Study. <i>Separation Science and Technology</i> , 2014, 49, 1215-1226.	2.5	6
97	Adsorption and separation of CO ₂ /CH ₄ mixtures using nanoporous adsorbents by molecular simulation. <i>Fluid Phase Equilibria</i> , 2014, 362, 227-234.	2.5	49
98	Grazing angle X-ray fluorescence from periodic structures on silicon and silica surfaces. <i>Spectrochimica Acta, Part B: Atomic Spectroscopy</i> , 2014, 98, 65-75.	2.9	17
99	Magnetic properties of the Cu-doped ZnO ^{1/4} experiments and theory. <i>Wuli Xuebao/Acta Physica Sinica</i> , 2014, 63, 157502.	0.5	5
100	High-energy-resolution grazing emission X-ray fluorescence applied to the characterization of thin Al films on Si. <i>Spectrochimica Acta, Part B: Atomic Spectroscopy</i> , 2013, 88, 136-149.	2.9	16
101	Magnetic Superatoms in VLi _n (n = 1-13) Clusters: A First-Principles Prediction. <i>Journal of Physical Chemistry A</i> , 2013, 117, 13025-13036.	2.5	38
102	The magnetic properties of Fe _x Zn _{1-x} O synthesized via the solid-state reaction route: Experiment and theory. <i>Journal of Magnetism and Magnetic Materials</i> , 2013, 340, 5-9.	2.3	24
103	Quantification of strain through linear dichroism in the Si 1s edge X-ray absorption spectra of strained Si _{1-x} Ge _x thin films. <i>Applied Surface Science</i> , 2013, 265, 358-362.	6.1	4
104	Ionic hydration of Na ⁺ inside carbon nanotubes, under electric fields. <i>Fluid Phase Equilibria</i> , 2013, 353, 1-6.	2.5	14
105	Dissociation of chloromethanes upon resonant ĩf* excitation studied by x-ray scattering. <i>Journal of Chemical Physics</i> , 2013, 139, 134302.	3.0	19
106	Depth profiling of dopants implanted in Si using the synchrotron radiation based high-resolution grazing emission technique. <i>X-Ray Spectrometry</i> , 2012, 41, 98-104.	1.4	16
107	Testing spatial noncommutativity via magnetic hyperfine structure induced by fractional angular momentum of Rydberg system. <i>Europhysics Letters</i> , 2012, 98, 40002.	2.0	2
108	Aqueous Dispersions of Few-Layered and Monolayered Hexagonal Boron Nitride Nanosheets from Sonication-Assisted Hydrolysis: Critical Role of Water. <i>Journal of Physical Chemistry C</i> , 2011, 115, 2679-2685.	3.1	519

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109	First Observation of Two-Electron One-Photon Transitions in Single-Photon K -Shell Double Ionization. <i>Physical Review Letters</i> , 2011, 107, 053001.	7.8	27
110	High-resolution KMM radiative Auger x-ray emission spectra of calcium induced by synchrotron radiation. <i>Physical Review A</i> , 2011, 83, .	2.5	4
111	Double L -shell photoionization of Pd induced by impact with medium-energy electrons. <i>Physical Review A</i> , 2011, 83, .	2.5	3
112	Resonant inelastic x-ray scattering at the limit of subfemtosecond natural lifetime. <i>Journal of Chemical Physics</i> , 2011, 134, 144308.	3.0	30
113	Double K -shell photoionization and hypersatellite x-ray transitions of ^{12}C . <i>Physical Review A</i> , 2010, 82, .	2.5	21
114	Depth profiles of Al impurities implanted in Si wafers determined by means of the high-resolution grazing emission X-ray fluorescence technique. <i>Spectrochimica Acta, Part B: Atomic Spectroscopy</i> , 2010, 65, 445-449.	2.9	14
115	Synchrotron-radiation-based determination of Xe L -subshell Coster-Kronig yields: A reexamination via high-resolution x-ray spectroscopy. <i>Physical Review A</i> , 2010, 81, .	2.5	8
116	Single-photon double K-shell ionization of low-Z atoms. <i>Journal of Physics: Conference Series</i> , 2010, 212, 012006.	0.4	1
117	Observation of ultralow-level Al impurities on a silicon surface by high-resolution grazing emission x-ray fluorescence excited by synchrotron radiation. <i>Physical Review B</i> , 2009, 80, .	3.2	21
118	Separation of Two-Electron Photoexcited Atomic Processes near the Inner-Shell Threshold. <i>Physical Review Letters</i> , 2009, 102, 143001.	7.8	32
119	Double K -shell ionization of Al induced by photon and electron impact. <i>Physical Review A</i> , 2009, 79, .	2.5	15
120	Application of the high-resolution grazing-emission x-ray fluorescence method for impurities control in semiconductor nanotechnology. <i>Journal of Applied Physics</i> , 2009, 105, 086101.	2.5	25
121	Double K -shell photoionization of low-Z atoms and He-like ions. <i>European Physical Journal: Special Topics</i> , 2009, 169, 23-27.	2.6	1
122	L -subshell Coster-Kronig yields of palladium determined via synchrotron-radiation-based high-resolution x-ray spectroscopy. <i>Physical Review A</i> , 2009, 80, .	2.5	7
123	Relative detection efficiency of back- and front-illuminated charge-coupled device cameras for x-rays between 1keV and 18keV. <i>Review of Scientific Instruments</i> , 2007, 78, 093102.	1.3	26
124	Chemical effects in the $K\alpha$ X-ray emission spectra of sulfur. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007, 260, 642-646.	1.4	28
125	Many-body calculation of helium $1D$ term intervals for $1s n d$ ($n=12$ to 20) high Rydberg states. <i>Canadian Journal of Physics</i> , 2006, 84, 1097-1106.	1.1	0