List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Temperature-dependent XPS studies on Ga-In alloys through the melting-point. Surface Science, 2022, 717, 122008.	1.9	4
2	Anchoring of porphyrins on atomically defined cobalt oxide: In-situ infrared spectroscopy at the electrified solid/liquid interface. Surface Science, 2022, 718, 122013.	1.9	1
3	Triggering the energy release in molecular solar thermal systems: Norbornadiene-functionalized trioxatriangulen on Au(111). Nano Energy, 2022, 95, 107007.	16.0	10
4	Reversible structural rearrangement of π-expanded cyclooctatetraene upon two-fold reduction with alkali metals. Chemical Communications, 2022, 58, 3206-3209.	4.1	9
5	Selektivitäskontrolle in elektrokatalytischen Oxidationsreaktionen durch Ionische FlÃ1⁄4ssigkeiten. Angewandte Chemie, 2022, 134, .	2.0	2
6	Modifying the Electrocatalytic Selectivity of Oxidation Reactions with Ionic Liquids. Angewandte Chemie - International Edition, 2022, 61, .	13.8	13
7	Supraparticles for Bareâ€Eye H ₂ Indication and Monitoring: Design, Working Principle, and Molecular Mobility (Adv. Funct. Mater. 22/2022). Advanced Functional Materials, 2022, 32, .	14.9	1
8	Surface Chemistry of the Molecular Solar Thermal Energy Storage System 2,3â€Dicyanoâ€Norbornadiene/Quadricyclane on Ni(111). ChemPhysChem, 2022, 23, .	2.1	7
9	Planar π-extended cycloparaphenylenes featuring an all-armchair edge topology. Nature Chemistry, 2022, 14, 871-876.	13.6	19
10	Reduction of Ï€â€Expanded Cyclooctatetraene with Lithium: Stabilization of the Tetraâ€Anion through Internal Li + Coordination. Angewandte Chemie, 2021, 133, 3552-3556.	2.0	10
11	Reduction of Ï€â€Expanded Cyclooctatetraene with Lithium: Stabilization of the Tetraâ€Anion through Internal Li ⁺ Coordination. Angewandte Chemie - International Edition, 2021, 60, 3510-3514.	13.8	17
12	Toward chemical accuracy at low computational cost: Density-functional theory with <i> <i>Ïf </i> /i>-functionals for the correlation energy. Journal of Chemical Physics, 2021, 154, 014104.</i>	3.0	19
13	An embedded atom model for Ga–Pd systems: From intermetallic crystals to liquid alloys. Journal of Chemical Physics, 2021, 154, 014109.	3.0	0
14	Screening Nanographeneâ€Mediated Inter(Porphyrin) Communication to Optimize Inter(Porphyrin–Fullerene) Forces. Advanced Energy Materials, 2021, 11, 2100158.	19.5	9
15	Controlling and Fine-Tuning Charge-Transfer Emission in 2,6-Dicyanoaniline Multichromophores Prepared through Domino Reactions: Entry to a Potentially New Class of OLEDs. Journal of Organic Chemistry, 2021, 86, 6111-6125.	3.2	7
16	A Molecular View of the Ionic Liquid Catalyst Interface of SCILLs: Coverage-Dependent Adsorption Motifs of [C ₄ C ₁ Pyr][NTf ₂] on Pd Single Crystals and Nanoparticles. Journal of Physical Chemistry C, 2021, 125, 13264-13272.	3.1	9
17	CO Permeability and Wetting Behavior of Ionic Liquids on Pt(111): An IRAS and PM-IRAS Study from Ultrahigh Vacuum to Ambient Pressure. Journal of Physical Chemistry C, 2021, 125, 15301-15315.	3.1	9
18	A Family of Superhelicenes: Easily Tunable, Chiral Nanographenes by Merging Helicity with Planar π Systems. Angewandte Chemie - International Edition, 2021, 60, 18073-18081.	13.8	48

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19	A Family of Superhelicenes: Easily Tunable, Chiral Nanographenes by Merging Helicity with Planar π Systems. Angewandte Chemie, 2021, 133, 18221-18229.	2.0	15
20	Numerically stable optimized effective potential method with standard Gaussian basis sets. Journal of Chemical Physics, 2021, 155, 054109.	3.0	8
21	Surface oxidation-induced restructuring of liquid Pd–Ga SCALMS model catalysts. Physical Chemistry Chemical Physics, 2021, 23, 16324-16333.	2.8	3
22	Chemical accuracy with <i>Ïf </i> -functionals for the Kohn–Sham correlation energy optimized for different input orbitals and eigenvalues. Journal of Chemical Physics, 2021, 155, 134111.	3.0	14
23	Adsorption Motifs and Molecular Orientation at the Ionic Liquid/Noble Metal Interface: [C ₂ C ₁ Im][NTf ₂] on Pt(111). Langmuir, 2021, 37, 12596-12607.	3.5	9
24	Oxidation induced restructuring of Rh–Ga SCALMS model catalyst systems. Journal of Chemical Physics, 2020, 153, 104702.	3.0	9
25	Analytic energy gradients for the self-consistent direct random phase approximation. Journal of Chemical Physics, 2020, 153, 134113.	3.0	7
26	Area‣elective Growth of HfS ₂ Thin Films via Atomic Layer Deposition at Low Temperature. Advanced Materials Interfaces, 2020, 7, 2001493.	3.7	10
27	Metalated Graphyne-Based Networks as Two-Dimensional Materials: Crystallization, Topological Defects, Delocalized Electronic States, and Site-Specific Doping. ACS Nano, 2020, 14, 16887-16896.	14.6	17
28	Thin Films: Area‧elective Growth of HfS ₂ Thin Films via Atomic Layer Deposition at Low Temperature (Adv. Mater. Interfaces 23/2020). Advanced Materials Interfaces, 2020, 7, 2070130.	3.7	0
29	Investigation of Cycloparaphenylenes (CPPs) and their Noncovalent Ringâ€inâ€Ring and Fullereneâ€inâ€Ring Complexes by (Matrixâ€Assisted) Laser Desorption/Ionization and Density Functional Theory. Chemistry - A European Journal, 2020, 26, 8729-8741.	3.3	23
30	Secondary Alcohols as Rechargeable Electrofuels: Electrooxidation of Isopropyl Alcohol at Pt Electrodes. ACS Catalysis, 2020, 10, 6831-6842.	11.2	32
31	Phosphorus ontaining Dibenzonaphthanthrenes: Electronic Fine Tuning of Polycyclic Aromatic Hydrocarbons through Organophosphorus Chemistry. Chemistry - A European Journal, 2020, 26, 13157-13162.	3.3	15
32	Analytic energy gradients for the exact exchange Kohn–Sham method. Journal of Chemical Physics, 2020, 152, 114113.	3.0	6
33	Lieb–Oxford bound and pair correlation functions for density-functional methods based on the adiabatic-connection fluctuation-dissipation theorem. Faraday Discussions, 2020, 224, 79-97.	3.2	1
34	On‣urface Assembly of Hydrogen―and Halogenâ€Bonded Supramolecular Graphyne‣ike Networks. Angewandte Chemie, 2020, 132, 9636-9642.	2.0	3
35	Onâ€Surface Assembly of Hydrogen―and Halogenâ€Bonded Supramolecular Graphyneâ€Like Networks. Angewandte Chemie - International Edition, 2020, 59, 9549-9555.	13.8	21
36	Explaining Cu@Pt Bimetallic Nanoparticles Activity Based on NO Adsorption. Chemistry - A European Journal, 2020, 26, 11478-11491.	3.3	5

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37	Norbornadiene photoswitches anchored to well-defined oxide surfaces: From ultrahigh vacuum into the liquid and the electrochemical environment. Journal of Chemical Physics, 2020, 152, 044708.	3.0	18
38	Controlled Catalytic Energy Release of the Norbornadiene/Quadricyclane Molecular Solar Thermal Energy Storage System on Ni(111). Journal of Physical Chemistry C, 2019, 123, 7654-7664.	3.1	25
39	Electrochemically controlled energy storage in a norbornadiene-based solar fuel with 99% reversibility. Nano Energy, 2019, 63, 103872.	16.0	31
40	Dehydrogenation of the liquid organic hydrogen carrier system 2-methylindole/2-methylindoline/2-methyloctahydroindole on Pt(111). Journal of Chemical Physics, 2019, 151, 144711.	3.0	19
41	Assessment of the exact-exchange-only Kohn-Sham method for the calculation of band structures for transition metal oxide and metal halide perovskites. Physical Review B, 2019, 100, .	3.2	5
42	Highly Effective Propane Dehydrogenation Using Ga–Rh Supported Catalytically Active Liquid Metal Solutions. ACS Catalysis, 2019, 9, 9499-9507.	11.2	76
43	Facile Access to Challenging <i>ortho</i> â€Terphenyls via Merging Two Multiâ€6tep Domino Reactions in Oneâ€Pot: A Joint Experimental/Theoretical Study. ChemCatChem, 2019, 11, 3982-3992.	3.7	8
44	Hierarchies of methods towards the exact Kohn-Sham correlation energy based on the adiabatic-connection fluctuation-dissipation theorem. Physical Review B, 2019, 99, .	3.2	35
45	Solar energy storage at an atomically defined organic-oxide hybrid interface. Nature Communications, 2019, 10, 2384.	12.8	37
46	Surface chemistry of 2,3-dibromosubstituted norbornadiene/quadricyclane as molecular solar thermal energy storage system on Ni(111). Journal of Chemical Physics, 2019, 150, 184706.	3.0	17
47	Oxygen Functionalization of Hexagonal Boron Nitride on Ni(111). Chemistry - A European Journal, 2019, 25, 8884-8893.	3.3	10
48	Operando DRIFTS and DFT Study of Propane Dehydrogenation over Solid- and Liquid-Supported Ga _{<i>x</i>} Pt _{<i>y</i>} Catalysts. ACS Catalysis, 2019, 9, 2842-2853.	11.2	83
49	Robust and accurate hybrid random-phase-approximation methods. Journal of Chemical Physics, 2019, 151, 144117.	3.0	12
50	Dynamic CO Adsorption and Desorption through the Ionic Liquid Layer of a Pt Model Solid Catalyst with Ionic Liquid Layers. Journal of Physical Chemistry C, 2019, 123, 31057-31072.	3.1	12
51	Pd-Ga model SCALMS: Characterization and stability of Pd single atom sites. Journal of Catalysis, 2019, 369, 33-46.	6.2	33
52	Topological Phase Transitions in Zinc-Blende Semimetals Driven Exclusively by Electronic Temperature. Physical Review Letters, 2018, 120, 146401.	7.8	2
53	Two-dimensional delocalized states in organometallic bis-acetylide networks on Ag(111). Nanoscale, 2018, 10, 3769-3776.	5.6	32
54	Phosphonic Acids on an Atomically Defined Oxide Surface: The Binding Motif Changes with Surface Coverage. Journal of Physical Chemistry Letters, 2018, 9, 1937-1943.	4.6	9

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55	Spin-current density-functional theory for a correct treatment of spin-orbit interactions and its application to topological phase transitions. Physical Review B, 2018, 98, .	3.2	18
56	Enforcing Extended Porphyrin J-Aggregate Stacking in Covalent Organic Frameworks. Journal of the American Chemical Society, 2018, 140, 16544-16552.	13.7	123
57	Solving the Puzzle of the Coexistence of Different Adsorption Geometries of Graphene on Ni(111). Journal of Physical Chemistry C, 2018, 122, 26105-26110.	3.1	9
58	Assessment of quality and reliability of band structures from exact-exchange-only Kohn–Sham, hybrid, and GW methods. European Physical Journal B, 2018, 91, 1.	1.5	2
59	Selective reduction of SWCNTs – concepts and insights. Journal of Materials Chemistry C, 2017, 5, 3937-3947.	5.5	10
60	ZnO Nanoparticle Formation from the Molecular Precursor [MeZnO <i>t</i> Bu] ₄ by Ozone Treatment in Ionic Liquids: inâ€situ Vibrational Spectroscopy in an Ultrahigh Vacuum Environment. Zeitschrift Fur Anorganische Und Allgemeine Chemie, 2017, 643, 31-40.	1.2	5
61	Understanding band gaps of solids in generalized Kohn–Sham theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2801-2806.	7.1	423
62	Coverage-Dependent Anchoring of 4,4′-Biphenyl Dicarboxylic Acid to CoO(111) Thin Films. Langmuir, 2017, 33, 4178-4188.	3.5	13
63	Deeper Insight into the Sixâ€Step Domino Reaction of Aldehydes with Malononitrile and Evaluation of Antiviral and Antimalarial Activities of the Obtained Bicyclic Products. ChemistryOpen, 2017, 6, 364-374.	1.9	5
64	Anchoring of a Carboxyl-Functionalized Norbornadiene Derivative to an Atomically Defined Cobalt Oxide Surface. Journal of Physical Chemistry C, 2017, 121, 11508-11518.	3.1	13
65	Catalytically Triggered Energy Release from Strained Organic Molecules: The Surface Chemistry of Quadricyclane and Norbornadiene on Pt(111). Chemistry - A European Journal, 2017, 23, 1613-1622.	3.3	31
66	Hierarchical on-surface synthesis and electronic structure of carbonyl-functionalized one- and two-dimensional covalent nanoarchitectures. Nature Communications, 2017, 8, 14765.	12.8	120
67	Spectroscopic Observation and Molecular Dynamics Simulation of Ga Surface Segregation in Liquid Pd–Ga Alloys. Chemistry - A European Journal, 2017, 23, 17701-17706.	3.3	19
68	Gallium-rich Pd–Ga phases as supported liquid metal catalysts. Nature Chemistry, 2017, 9, 862-867.	13.6	234
69	Model Catalytic Studies of Novel Liquid Organic Hydrogen Carriers: Indole, Indoline and Octahydroindole on Pt(111). Chemistry - A European Journal, 2017, 23, 14806-14818.	3.3	24
70	Accurate Valence Ionization Energies from Kohn–Sham Eigenvalues with the Help of Potential Adjustors. Journal of Chemical Theory and Computation, 2017, 13, 4726-4740.	5.3	11
71	Hydrogenation and hydrogen intercalation of hexagonal boron nitride on Ni(1 1 1): reactivity and electronic structure. 2D Materials, 2017, 4, 035026.	4.4	28
72	Palladiumâ€Mediated Ethylation of the Imidazolium Cation Monitored In Operando on a Solid Catalyst with Ionic Liquid Layer. ChemCatChem, 2017, 9, 109-113.	3.7	14

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73	Frontispiece: Spectroscopic Observation and Molecular Dynamics Simulation of Ga Surface Segregation in Liquid Pd–Ga Alloys. Chemistry - A European Journal, 2017, 23, .	3.3	0
74	Power Series Approximation for the Correlation Kernel Leading to Kohn-Sham Methods Combining Accuracy, Computational Efficiency, and General Applicability. Physical Review Letters, 2016, 117, 143002.	7.8	57
75	Band gaps, ionization potentials, and electron affinities of periodic electron systems via the adiabatic-connection fluctuation-dissipation theorem. Physical Review B, 2016, 94, .	3.2	16
76	The contact of graphene with Ni(111) surface: description by modern dispersive forces approaches. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	15
77	Energy Storage in Strained Organic Molecules: (Spectro)Electrochemical Characterization of Norbornadiene and Quadricyclane. ChemSusChem, 2016, 9, 1424-1432.	6.8	55
78	Generation of Complex Azabicycles and Carbobicycles from Two Simple Compounds in a Single Operation through a Metalâ€Free Sixâ€Step Domino Reaction. Chemistry - A European Journal, 2016, 22, 5189-5197.	3.3	14
79	Exchange-correlation potentials with proper discontinuities for physically meaningful Kohn-Sham eigenvalues and band structures. Physical Review B, 2015, 91, .	3.2	50
80	Self-consistent Kohn-Sham method based on the adiabatic-connection fluctuation-dissipation theorem and the exact-exchange kernel. Journal of Chemical Physics, 2015, 142, 244108.	3.0	39
81	Molecular Orientation and Structural Transformations in Phthalic Anhydride Thin Films on MgO(100)/Ag(100). Langmuir, 2015, 31, 7806-7814.	3.5	16
82	Supported homogeneous catalyst makes its own liquid phase. Journal of Catalysis, 2015, 321, 32-38.	6.2	27
83	High Resolution Scanning Tunneling Microscopy of a 1D Coordination Polymer with Imidazoleâ€Based <i>N,N,O</i> Ligands on HOPG. Chemistry - A European Journal, 2014, 20, 11863-11869.	3.3	5
84	Stability conditions for exact-exchange Kohn-Sham methods and their relation to correlation energies from the adiabatic-connection fluctuation-dissipation theorem. Journal of Chemical Physics, 2014, 141, 204107.	3.0	10
85	Michael Addition of Nâ€Unprotected 2â€Oxindoles to Nitrostyrene Catalyzed by Bifunctional Tertiary Amines: Crucial Role of Dispersion Interactions. ChemCatChem, 2014, 6, 1324-1332.	3.7	13
86	Efficient self-consistent treatment of electron correlation within the random phase approximation. Journal of Chemical Physics, 2013, 139, 084113.	3.0	81
87	Influence of the exchange-correlation potential in methods based on time-dependent density-functional theory. Physical Review A, 2013, 88, .	2.5	15
88	Directional Noncovalent Interactions: Repulsion and Dispersion. Journal of Chemical Theory and Computation, 2013, 9, 2264-2275.	5.3	64
89	Dehydrogenation Mechanism of Liquid Organic Hydrogen Carriers: Dodecahydroâ€ <i>N</i> â€ethylcarbazole on Pd(111). Chemistry - A European Journal, 2013, 19, 10854-10865.	3.3	79
90	Influence of the surface dipole layer and Pauli repulsion on band energies and doping in graphene adsorbed on metal surfaces. Physical Review B, 2012, 86, .	3.2	35

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91	Bonding Mechanisms of Graphene on Metal Surfaces. Journal of Physical Chemistry C, 2012, 116, 7360-7366.	3.1	133
92	Preparation and characterization of ultrathin [Ru(CO)3Cl2]2 and [BMIM][Tf2N] films on Al2O3/NiAl(110) under UHV conditions. Physical Chemistry Chemical Physics, 2012, 14, 10603.	2.8	15
93	Competition for Graphene: Graphynes with Direction-Dependent Dirac Cones. Physical Review Letters, 2012, 108, 086804.	7.8	995
94	Precise response functions in all-electron methods: Application to the optimized-effective-potential approach. Physical Review B, 2012, 85, .	3.2	43
95	Resolution of identity approach for the Kohn-Sham correlation energy within the exact-exchange random-phase approximation. Journal of Chemical Physics, 2012, 136, 134102.	3.0	52
96	Local exact exchange potentials within the all-electron FLAPW method and a comparison with pseudopotential results. Physical Review B, 2011, 83, .	3.2	49
97	Correct Description of the Bond Dissociation Limit without Breaking Spin Symmetry by a Random-Phase-Approximation Correlation Functional. Physical Review Letters, 2011, 106, 093001.	7.8	106
98	Graphene on Ni(111): Coexistence of Different Surface Structures. Journal of Physical Chemistry Letters, 2011, 2, 759-764.	4.6	158
99	Random-phase approximation correlation methods for molecules and solids. Molecular Physics, 2011, 109, 2473-2500.	1.7	146
100	Dehydrogenation of Dodecahydroâ€ <i>N</i> â€ethylcarbazole on Pd/Al ₂ O ₃ Model Catalysts. Chemistry - A European Journal, 2011, 17, 11542-11552.	3.3	89
101	Efficient exact-exchange time-dependent density-functional theory methods and their relation to time-dependent Hartree–Fock. Journal of Chemical Physics, 2011, 134, 034120.	3.0	25
102	Methane Activation by Platinum: Critical Role of Edge and Corner Sites of Metal Nanoparticles. Chemistry - A European Journal, 2010, 16, 6530-6539.	3.3	126
103	Molecular excitation spectra by TDDFT with the nonadiabatic exact exchange kernel. International Journal of Quantum Chemistry, 2010, 110, 2202-2220.	2.0	23
104	Density-Functional Theory with Orbital-Dependent Functionals: Exact-exchange Kohn-Sham and Density-Functional Response Methods. Zeitschrift Fur Physikalische Chemie, 2010, 224, 325-342.	2.8	16
105	Random phase approximation correlation energies with exact Kohn–Sham exchange. Molecular Physics, 2010, 108, 359-372.	1.7	121
106	Extension of exact-exchange density functional theory of solids to finite temperatures. Physical Review B, 2010, 81, .	3.2	20
107	Toward Ionic-Liquid-Based Model Catalysis: Growth, Orientation, Conformation, and Interaction Mechanism of the [Tf ₂ N] ^{â^'} Anion in [BMIM][Tf ₂ N] Thin Films on a Well-Ordered Alumina Surface. Langmuir, 2010, 26, 7199-7207.	3.5	116
108	Density Functional Calculations and IR Reflection Absorption Spectroscopy on the Interaction of SO ₂ with Oxide-Supported Pd Nanoparticles. Journal of Physical Chemistry C, 2010, 114, 13813-13824.	3.1	20

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109	A Combined Density-Functional and IRAS Study on the Interaction of NO with Pd Nanoparticles: Identifying New Adsorption Sites with Novel Properties. Journal of Physical Chemistry C, 2008, 112, 16539-16549.	3.1	41
110	Relation between exchange-only optimized potential and Kohn–Sham methods with finite basis sets, and effect of linearly dependent products of orbital basis functions. Journal of Chemical Physics, 2008, 128, 104104.	3.0	61
111	Numerically stable optimized effective potential method with balanced Gaussian basis sets. Journal of Chemical Physics, 2007, 127, 054102.	3.0	130
112	Exact-Exchange Spin-Current Density-Functional Theory. Physical Review Letters, 2006, 97, 013005.	7.8	33
113	Orbital- and state-dependent functionals in density-functional theory. Journal of Chemical Physics, 2005, 123, 062203.	3.0	125
114	Asymptotic Behavior of the Kohn-Sham Exchange Potential. Physical Review Letters, 2002, 89, 033003.	7.8	105
115	Exact Kohn-Sham exchange kernel for insulators and its long-wavelength behavior. Physical Review B, 2002, 66, .	3.2	71
116	Efficient localized Hartree–Fock methods as effective exact-exchange Kohn–Sham methods for molecules. Journal of Chemical Physics, 2001, 115, 5718-5732.	3.0	319
117	Exact exchange Kohn-Sham formalism applied to semiconductors. Physical Review B, 1999, 59, 10031-10043.	3.2	358
118	New KS Method for Molecules Based on an Exchange Charge Density Generating the Exact Local KS Exchange Potential. Physical Review Letters, 1999, 83, 5459-5462.	7.8	340
119	Exact exchange kernel for time-dependent density-functional theory. International Journal of Quantum Chemistry, 1998, 69, 265-277.	2.0	81
120	Exact exchange-correlation kernel for dynamic response properties and excitation energies in density-functional theory. Physical Review A, 1998, 57, 3433-3436.	2.5	74
121	Exact exchange kernel for time-dependent density-functional theory. , 1998, 69, 265.		13
122	Time-dependent Kohn-Sham formalism. Physical Review A, 1997, 55, 2630-2639.	2.5	39
123	Exact Kohn-Sham Exchange Potential in Semiconductors. Physical Review Letters, 1997, 79, 2089-2092.	7.8	329
124	Exact treatment of exchange in Kohn-Sham band-structure schemes. Physical Review B, 1996, 53, 7024-7029.	3.2	89
125	Generalized Kohn-Sham schemes and the band-gap problem. Physical Review B, 1996, 53, 3764-3774.	3.2	1,075
126	DFT ionization formulas and aDFT perturbation theory for exchange and correlation, through adiabatic connection. International Journal of Quantum Chemistry, 1995, 56, 93-108.	2.0	142

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127	Energy differences between Kohn-Sham and Hartree-Fock wave functions yielding the same electron density. Physical Review A, 1995, 51, 4501-4513.	2.5	126
128	Hardness of molecules and the band gap of solids within the Kohn-Sham formalism: A perturbation-scaling approach. Physical Review A, 1995, 52, 4493-4499.	2.5	74
129	Exact Kohn-Sham scheme based on perturbation theory. Physical Review A, 1994, 50, 196-204.	2.5	506
130	Symmetry in density-functional theory. Physical Review A, 1993, 47, 2783-2799.	2.5	126
131	Correlation-energy functional and its high-density limit obtained from a coupling-constant perturbation expansion. Physical Review B, 1993, 47, 13105-13113.	3.2	385
132	Kohn-Sham potentials and wave functions from electron densities. Physical Review A, 1992, 46, 3753-3757.	2.5	109
133	Numerically stable inversion approach to construct Kohn-Sham potentials for given electron densities within a Gaussian basis set framework. Journal of Chemical Physics, O	3.0	1