

# Andreas Gärting

## List of Publications by Year in descending order

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133  
papers

9,584  
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61984

43  
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37204

96  
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136  
all docs

136  
docs citations

136  
times ranked

7273  
citing authors

#	ARTICLE	IF	CITATIONS
1	Generalized Kohn-Sham schemes and the band-gap problem. <i>Physical Review B</i> , 1996, 53, 3764-3774.	3.2	1,075
2	Competition for Graphene: Graphynes with Direction-Dependent Dirac Cones. <i>Physical Review Letters</i> , 2012, 108, 086804.	7.8	995
3	Exact Kohn-Sham scheme based on perturbation theory. <i>Physical Review A</i> , 1994, 50, 196-204.	2.5	506
4	Understanding band gaps of solids in generalized Kohn-Sham theory. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 2801-2806.	7.1	423
5	Correlation-energy functional and its high-density limit obtained from a coupling-constant perturbation expansion. <i>Physical Review B</i> , 1993, 47, 13105-13113.	3.2	385
6	Exact exchange Kohn-Sham formalism applied to semiconductors. <i>Physical Review B</i> , 1999, 59, 10031-10043.	3.2	358
7	New KS Method for Molecules Based on an Exchange Charge Density Generating the Exact Local KS Exchange Potential. <i>Physical Review Letters</i> , 1999, 83, 5459-5462.	7.8	340
8	Exact Kohn-Sham Exchange Potential in Semiconductors. <i>Physical Review Letters</i> , 1997, 79, 2089-2092.	7.8	329
9	Efficient localized Hartree-Fock methods as effective exact-exchange Kohn-Sham methods for molecules. <i>Journal of Chemical Physics</i> , 2001, 115, 5718-5732.	3.0	319
10	Gallium-rich Pd-Ga phases as supported liquid metal catalysts. <i>Nature Chemistry</i> , 2017, 9, 862-867.	13.6	234
11	Graphene on Ni(111): Coexistence of Different Surface Structures. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 759-764.	4.6	158
12	Random-phase approximation correlation methods for molecules and solids. <i>Molecular Physics</i> , 2011, 109, 2473-2500.	1.7	146
13	DFT ionization formulas and aDFT perturbation theory for exchange and correlation, through adiabatic connection. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 93-108.	2.0	142
14	Bonding Mechanisms of Graphene on Metal Surfaces. <i>Journal of Physical Chemistry C</i> , 2012, 116, 7360-7366.	3.1	133
15	Numerically stable optimized effective potential method with balanced Gaussian basis sets. <i>Journal of Chemical Physics</i> , 2007, 127, 054102.	3.0	130
16	Symmetry in density-functional theory. <i>Physical Review A</i> , 1993, 47, 2783-2799.	2.5	126
17	Energy differences between Kohn-Sham and Hartree-Fock wave functions yielding the same electron density. <i>Physical Review A</i> , 1995, 51, 4501-4513.	2.5	126
18	Methane Activation by Platinum: Critical Role of Edge and Corner Sites of Metal Nanoparticles. <i>Chemistry - A European Journal</i> , 2010, 16, 6530-6539.	3.3	126

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19	Orbital- and state-dependent functionals in density-functional theory. <i>Journal of Chemical Physics</i> , 2005, 123, 062203.	3.0	125
20	Enforcing Extended Porphyrin J-Aggregate Stacking in Covalent Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2018, 140, 16544-16552.	13.7	123
21	Random phase approximation correlation energies with exact Kohn-Sham exchange. <i>Molecular Physics</i> , 2010, 108, 359-372.	1.7	121
22	Hierarchical on-surface synthesis and electronic structure of carbonyl-functionalized one- and two-dimensional covalent nanoarchitectures. <i>Nature Communications</i> , 2017, 8, 14765.	12.8	120
23	Toward Ionic-Liquid-Based Model Catalysis: Growth, Orientation, Conformation, and Interaction Mechanism of the $[Tf_2N]^+$ Anion in $[BMIM][Tf_2N]$ Thin Films on a Well-Ordered Alumina Surface. <i>Langmuir</i> , 2010, 26, 7199-7207.	3.5	116
24	Kohn-Sham potentials and wave functions from electron densities. <i>Physical Review A</i> , 1992, 46, 3753-3757.	2.5	109
25	Correct Description of the Bond Dissociation Limit without Breaking Spin Symmetry by a Random-Phase-Approximation Correlation Functional. <i>Physical Review Letters</i> , 2011, 106, 093001.	7.8	106
26	Asymptotic Behavior of the Kohn-Sham Exchange Potential. <i>Physical Review Letters</i> , 2002, 89, 033003.	7.8	105
27	Exact treatment of exchange in Kohn-Sham band-structure schemes. <i>Physical Review B</i> , 1996, 53, 7024-7029.	3.2	89
28	Dehydrogenation of Dodecahydro- <i>N</i> -ethylcarbazole on Pd/Al <sub>2</sub> O <sub>3</sub> Model Catalysts. <i>Chemistry - A European Journal</i> , 2011, 17, 11542-11552.	3.3	89
29	Operando DRIFTS and DFT Study of Propane Dehydrogenation over Solid- and Liquid-Supported Ga <sub>x</sub> Pt <sub>y</sub> Catalysts. <i>ACS Catalysis</i> , 2019, 9, 2842-2853.	11.2	83
30	Exact exchange kernel for time-dependent density-functional theory. <i>International Journal of Quantum Chemistry</i> , 1998, 69, 265-277.	2.0	81
31	Efficient self-consistent treatment of electron correlation within the random phase approximation. <i>Journal of Chemical Physics</i> , 2013, 139, 084113.	3.0	81
32	Dehydrogenation Mechanism of Liquid Organic Hydrogen Carriers: Dodecahydro- <i>N</i> -ethylcarbazole on Pd(111). <i>Chemistry - A European Journal</i> , 2013, 19, 10854-10865.	3.3	79
33	Highly Effective Propane Dehydrogenation Using Ga-Rh Supported Catalytically Active Liquid Metal Solutions. <i>ACS Catalysis</i> , 2019, 9, 9499-9507.	11.2	76
34	Hardness of molecules and the band gap of solids within the Kohn-Sham formalism: A perturbation-scaling approach. <i>Physical Review A</i> , 1995, 52, 4493-4499.	2.5	74
35	Exact exchange-correlation kernel for dynamic response properties and excitation energies in density-functional theory. <i>Physical Review A</i> , 1998, 57, 3433-3436.	2.5	74
36	Exact Kohn-Sham exchange kernel for insulators and its long-wavelength behavior. <i>Physical Review B</i> , 2002, 66, .	3.2	71

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37	Directional Noncovalent Interactions: Repulsion and Dispersion. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2264-2275.	5.3	64
38	Relation between exchange-only optimized potential and Kohn-Sham methods with finite basis sets, and effect of linearly dependent products of orbital basis functions. <i>Journal of Chemical Physics</i> , 2008, 128, 104104.	3.0	61
39	Power Series Approximation for the Correlation Kernel Leading to Kohn-Sham Methods Combining Accuracy, Computational Efficiency, and General Applicability. <i>Physical Review Letters</i> , 2016, 117, 143002.	7.8	57
40	Energy Storage in Strained Organic Molecules: (Spectro)Electrochemical Characterization of Norbornadiene and Quadricyclane. <i>ChemSusChem</i> , 2016, 9, 1424-1432.	6.8	55
41	Resolution of identity approach for the Kohn-Sham correlation energy within the exact-exchange random-phase approximation. <i>Journal of Chemical Physics</i> , 2012, 136, 134102.	3.0	52
42	Exchange-correlation potentials with proper discontinuities for physically meaningful Kohn-Sham eigenvalues and band structures. <i>Physical Review B</i> , 2015, 91, .	3.2	50
43	Local exact exchange potentials within the all-electron FLAPW method and a comparison with pseudopotential results. <i>Physical Review B</i> , 2011, 83, .	3.2	49
44	A Family of Superhelicenes: Easily Tunable, Chiral Nanographenes by Merging Helicity with Planar $\pi$ Systems. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 18073-18081.	13.8	48
45	Precise response functions in all-electron methods: Application to the optimized-effective-potential approach. <i>Physical Review B</i> , 2012, 85, .	3.2	43
46	A Combined Density-Functional and IRAS Study on the Interaction of NO with Pd Nanoparticles: Identifying New Adsorption Sites with Novel Properties. <i>Journal of Physical Chemistry C</i> , 2008, 112, 16539-16549.	3.1	41
47	Time-dependent Kohn-Sham formalism. <i>Physical Review A</i> , 1997, 55, 2630-2639.	2.5	39
48	Self-consistent Kohn-Sham method based on the adiabatic-connection fluctuation-dissipation theorem and the exact-exchange kernel. <i>Journal of Chemical Physics</i> , 2015, 142, 244108.	3.0	39
49	Solar energy storage at an atomically defined organic-oxide hybrid interface. <i>Nature Communications</i> , 2019, 10, 2384.	12.8	37
50	Influence of the surface dipole layer and Pauli repulsion on band energies and doping in graphene adsorbed on metal surfaces. <i>Physical Review B</i> , 2012, 86, .	3.2	35
51	Hierarchies of methods towards the exact Kohn-Sham correlation energy based on the adiabatic-connection fluctuation-dissipation theorem. <i>Physical Review B</i> , 2019, 99, .	3.2	35
52	Exact-Exchange Spin-Current Density-Functional Theory. <i>Physical Review Letters</i> , 2006, 97, 013005.	7.8	33
53	Pd-Ga model SCALMS: Characterization and stability of Pd single atom sites. <i>Journal of Catalysis</i> , 2019, 369, 33-46.	6.2	33
54	Two-dimensional delocalized states in organometallic bis-acetylide networks on Ag(111). <i>Nanoscale</i> , 2018, 10, 3769-3776.	5.6	32

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55	Secondary Alcohols as Rechargeable Electrofuels: Electrooxidation of Isopropyl Alcohol at Pt Electrodes. <i>ACS Catalysis</i> , 2020, 10, 6831-6842.	11.2	32
56	Catalytically Triggered Energy Release from Strained Organic Molecules: The Surface Chemistry of Quadricyclane and Norbornadiene on Pt(111). <i>Chemistry - A European Journal</i> , 2017, 23, 1613-1622.	3.3	31
57	Electrochemically controlled energy storage in a norbornadiene-based solar fuel with 99% reversibility. <i>Nano Energy</i> , 2019, 63, 103872.	16.0	31
58	Hydrogenation and hydrogen intercalation of hexagonal boron nitride on Ni(111): reactivity and electronic structure. <i>2D Materials</i> , 2017, 4, 035026.	4.4	28
59	Supported homogeneous catalyst makes its own liquid phase. <i>Journal of Catalysis</i> , 2015, 321, 32-38.	6.2	27
60	Efficient exact-exchange time-dependent density-functional theory methods and their relation to time-dependent Hartree-Fock. <i>Journal of Chemical Physics</i> , 2011, 134, 034120.	3.0	25
61	Controlled Catalytic Energy Release of the Norbornadiene/Quadricyclane Molecular Solar Thermal Energy Storage System on Ni(111). <i>Journal of Physical Chemistry C</i> , 2019, 123, 7654-7664.	3.1	25
62	Model Catalytic Studies of Novel Liquid Organic Hydrogen Carriers: Indole, Indoline and Octahydroindole on Pt(111). <i>Chemistry - A European Journal</i> , 2017, 23, 14806-14818.	3.3	24
63	Molecular excitation spectra by TDDFT with the nonadiabatic exact exchange kernel. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2202-2220.	2.0	23
64	Investigation of Cycloparaphenylenes (CPPs) and their Noncovalent Ring-Ring and Fullerene-Ring Complexes by (Matrix-Assisted) Laser Desorption/Ionization and Density Functional Theory. <i>Chemistry - A European Journal</i> , 2020, 26, 8729-8741.	3.3	23
65	On-Surface Assembly of Hydrogen- and Halogen-Bonded Supramolecular Graphyne-Like Networks. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 9549-9555.	13.8	21
66	Extension of exact-exchange density functional theory of solids to finite temperatures. <i>Physical Review B</i> , 2010, 81, .	3.2	20
67	Density Functional Calculations and IR Reflection Absorption Spectroscopy on the Interaction of SO <sub>2</sub> with Oxide-Supported Pd Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2010, 114, 13813-13824.	3.1	20
68	Spectroscopic Observation and Molecular Dynamics Simulation of Ga Surface Segregation in Liquid Pd-Ga Alloys. <i>Chemistry - A European Journal</i> , 2017, 23, 17701-17706.	3.3	19
69	Dehydrogenation of the liquid organic hydrogen carrier system 2-methylindole/2-methylindoline/2-methyloctahydroindole on Pt(111). <i>Journal of Chemical Physics</i> , 2019, 151, 144711.	3.0	19
70	Toward chemical accuracy at low computational cost: Density-functional theory with $\tilde{f}$ -functionals for the correlation energy. <i>Journal of Chemical Physics</i> , 2021, 154, 014104.	3.0	19
71	Planar $\pi$ -extended cycloparaphenylenes featuring an all-armchair edge topology. <i>Nature Chemistry</i> , 2022, 14, 871-876.	13.6	19
72	Spin-current density-functional theory for a correct treatment of spin-orbit interactions and its application to topological phase transitions. <i>Physical Review B</i> , 2018, 98, .	3.2	18

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73	Norbornadiene photoswitches anchored to well-defined oxide surfaces: From ultrahigh vacuum into the liquid and the electrochemical environment. <i>Journal of Chemical Physics</i> , 2020, 152, 044708.	3.0	18
74	Surface chemistry of 2,3-dibromosubstituted norbornadiene/quadricyclane as molecular solar thermal energy storage system on Ni(111). <i>Journal of Chemical Physics</i> , 2019, 150, 184706.	3.0	17
75	Metalated Graphyne-Based Networks as Two-Dimensional Materials: Crystallization, Topological Defects, Delocalized Electronic States, and Site-Specific Doping. <i>ACS Nano</i> , 2020, 14, 16887-16896.	14.6	17
76	Reduction of $\text{Li}^+\text{C}_8\text{H}_6\text{O}^-$ Expanded Cyclooctatetraene with Lithium: Stabilization of the Tetraanion through Internal $\text{Li}^+$ Coordination. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 3510-3514.	13.8	17
77	Density-Functional Theory with Orbital-Dependent Functionals: Exact-exchange Kohn-Sham and Density-Functional Response Methods. <i>Zeitschrift Fur Physikalische Chemie</i> , 2010, 224, 325-342.	2.8	16
78	Molecular Orientation and Structural Transformations in Phthalic Anhydride Thin Films on MgO(100)/Ag(100). <i>Langmuir</i> , 2015, 31, 7806-7814.	3.5	16
79	Band gaps, ionization potentials, and electron affinities of periodic electron systems via the adiabatic-connection fluctuation-dissipation theorem. <i>Physical Review B</i> , 2016, 94, .	3.2	16
80	Preparation and characterization of ultrathin $[\text{Ru}(\text{CO})_3\text{Cl}_2]_2$ and $[\text{BMIM}][\text{Tf}_2\text{N}]$ films on $\text{Al}_2\text{O}_3/\text{NiAl}(110)$ under UHV conditions. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 10603.	2.8	15
81	Influence of the exchange-correlation potential in methods based on time-dependent density-functional theory. <i>Physical Review A</i> , 2013, 88, .	2.5	15
82	The contact of graphene with Ni(111) surface: description by modern dispersive forces approaches. <i>Theoretical Chemistry Accounts</i> , 2016, 135, 1.	1.4	15
83	Phosphorus-Containing Dibenzonaphthanthrenes: Electronic Fine Tuning of Polycyclic Aromatic Hydrocarbons through Organophosphorus Chemistry. <i>Chemistry - A European Journal</i> , 2020, 26, 13157-13162.	3.3	15
84	A Family of Superhelicenes: Easily Tunable, Chiral Nanographenes by Merging Helicity with Planar $\text{C}_6\text{H}_6$ Systems. <i>Angewandte Chemie</i> , 2021, 133, 18221-18229.	2.0	15
85	Generation of Complex Azabicycles and Carbobicycles from Two Simple Compounds in a Single Operation through a Metal-Free Six-Step Domino Reaction. <i>Chemistry - A European Journal</i> , 2016, 22, 5189-5197.	3.3	14
86	Palladium-Mediated Ethylation of the Imidazolium Cation Monitored In Operando on a Solid Catalyst with Ionic Liquid Layer. <i>ChemCatChem</i> , 2017, 9, 109-113.	3.7	14
87	Chemical accuracy with $\text{r}^2\text{SCAN}$ -functionals for the Kohn-Sham correlation energy optimized for different input orbitals and eigenvalues. <i>Journal of Chemical Physics</i> , 2021, 155, 134111.	3.0	14
88	Michael Addition of $\text{N}$ -Unprotected 2-Oxindoles to Nitrostyrene Catalyzed by Bifunctional Tertiary Amines: Crucial Role of Dispersion Interactions. <i>ChemCatChem</i> , 2014, 6, 1324-1332.	3.7	13
89	Coverage-Dependent Anchoring of 4,4'-Biphenyl Dicarboxylic Acid to $\text{CoO}(111)$ Thin Films. <i>Langmuir</i> , 2017, 33, 4178-4188.	3.5	13
90	Anchoring of a Carboxyl-Functionalized Norbornadiene Derivative to an Atomically Defined Cobalt Oxide Surface. <i>Journal of Physical Chemistry C</i> , 2017, 121, 11508-11518.	3.1	13

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91	Exact exchange kernel for time-dependent density-functional theory. , 1998, 69, 265.		13
92	Modifying the Electrocatalytic Selectivity of Oxidation Reactions with Ionic Liquids. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	13
93	Robust and accurate hybrid random-phase-approximation methods. <i>Journal of Chemical Physics</i> , 2019, 151, 144117.	3.0	12
94	Dynamic CO Adsorption and Desorption through the Ionic Liquid Layer of a Pt Model Solid Catalyst with Ionic Liquid Layers. <i>Journal of Physical Chemistry C</i> , 2019, 123, 31057-31072.	3.1	12
95	Accurate Valence Ionization Energies from Kohn-Sham Eigenvalues with the Help of Potential Adjustors. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4726-4740.	5.3	11
96	Stability conditions for exact-exchange Kohn-Sham methods and their relation to correlation energies from the adiabatic-connection fluctuation-dissipation theorem. <i>Journal of Chemical Physics</i> , 2014, 141, 204107.	3.0	10
97	Selective reduction of SWCNTs – concepts and insights. <i>Journal of Materials Chemistry C</i> , 2017, 5, 3937-3947.	5.5	10
98	Oxygen Functionalization of Hexagonal Boron Nitride on Ni(111). <i>Chemistry - A European Journal</i> , 2019, 25, 8884-8893.	3.3	10
99	Area-Selective Growth of HfO <sub>2</sub> Thin Films via Atomic Layer Deposition at Low Temperature. <i>Advanced Materials Interfaces</i> , 2020, 7, 2001493.	3.7	10
100	Reduction of –Expanded Cyclooctatetraene with Lithium: Stabilization of the Tetra-Anion through Internal Li + Coordination. <i>Angewandte Chemie</i> , 2021, 133, 3552-3556.	2.0	10
101	Triggering the energy release in molecular solar thermal systems: Norbornadiene-functionalized trioxatriangulen on Au(111). <i>Nano Energy</i> , 2022, 95, 107007.	16.0	10
102	Phosphonic Acids on an Atomically Defined Oxide Surface: The Binding Motif Changes with Surface Coverage. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1937-1943.	4.6	9
103	Solving the Puzzle of the Coexistence of Different Adsorption Geometries of Graphene on Ni(111). <i>Journal of Physical Chemistry C</i> , 2018, 122, 26105-26110.	3.1	9
104	Oxidation induced restructuring of Rh-Ga SCALMS model catalyst systems. <i>Journal of Chemical Physics</i> , 2020, 153, 104702.	3.0	9
105	Screening Nanographene-Mediated Inter(Porphyrin) Communication to Optimize Inter(Porphyrin-Fullerene) Forces. <i>Advanced Energy Materials</i> , 2021, 11, 2100158.	19.5	9
106	A Molecular View of the Ionic Liquid Catalyst Interface of SCILLs: Coverage-Dependent Adsorption Motifs of [C <sub>4</sub> C <sub>1</sub> Pyr][NTf <sub>2</sub> ] on Pd Single Crystals and Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2021, 125, 13264-13272.	3.1	9
107	CO Permeability and Wetting Behavior of Ionic Liquids on Pt(111): An IRAS and PM-IRAS Study from Ultrahigh Vacuum to Ambient Pressure. <i>Journal of Physical Chemistry C</i> , 2021, 125, 15301-15315.	3.1	9
108	Adsorption Motifs and Molecular Orientation at the Ionic Liquid/Noble Metal Interface: [C <sub>2</sub> C <sub>1</sub> Im][NTf <sub>2</sub> ] on Pt(111). <i>Langmuir</i> , 2021, 37, 12596-12607.	3.5	9

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109	Reversible structural rearrangement of $\pi$ -expanded cyclooctatetraene upon two-fold reduction with alkali metals. <i>Chemical Communications</i> , 2022, 58, 3206-3209.	4.1	9
110	Facile Access to Challenging <i>ortho</i> - <i>terphenyls</i> via Merging Two Multi-Step Domino Reactions in One-Pot: A Joint Experimental/Theoretical Study. <i>ChemCatChem</i> , 2019, 11, 3982-3992.	3.7	8
111	Numerically stable optimized effective potential method with standard Gaussian basis sets. <i>Journal of Chemical Physics</i> , 2021, 155, 054109.	3.0	8
112	Analytic energy gradients for the self-consistent direct random phase approximation. <i>Journal of Chemical Physics</i> , 2020, 153, 134113.	3.0	7
113	Controlling and Fine-Tuning Charge-Transfer Emission in 2,6-Dicyanoaniline Multichromophores Prepared through Domino Reactions: Entry to a Potentially New Class of OLEDs. <i>Journal of Organic Chemistry</i> , 2021, 86, 6111-6125.	3.2	7
114	Surface Chemistry of the Molecular Solar Thermal Energy Storage System 2,3-Dicyano-Norbornadiene/Quadricyclane on Ni(111). <i>ChemPhysChem</i> , 2022, 23, .	2.1	7
115	Analytic energy gradients for the exact exchange Kohn-Sham method. <i>Journal of Chemical Physics</i> , 2020, 152, 114113.	3.0	6
116	High Resolution Scanning Tunneling Microscopy of a 1D Coordination Polymer with Imidazole-Based <i>N,N,O</i> Ligands on HOPG. <i>Chemistry - A European Journal</i> , 2014, 20, 11863-11869.	3.3	5
117	ZnO Nanoparticle Formation from the Molecular Precursor $[\text{MeZnO}(\text{tBu})_4]$ by Ozone Treatment in Ionic Liquids: <i>in situ</i> Vibrational Spectroscopy in an Ultrahigh Vacuum Environment. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2017, 643, 31-40.	1.2	5
118	Deeper Insight into the Six-Step Domino Reaction of Aldehydes with Malononitrile and Evaluation of Antiviral and Antimalarial Activities of the Obtained Bicyclic Products. <i>ChemistryOpen</i> , 2017, 6, 364-374.	1.9	5
119	Assessment of the exact-exchange-only Kohn-Sham method for the calculation of band structures for transition metal oxide and metal halide perovskites. <i>Physical Review B</i> , 2019, 100, .	3.2	5
120	Explaining Cu@Pt Bimetallic Nanoparticles Activity Based on NO Adsorption. <i>Chemistry - A European Journal</i> , 2020, 26, 11478-11491.	3.3	5
121	Temperature-dependent XPS studies on Ga-In alloys through the melting-point. <i>Surface Science</i> , 2022, 717, 122008.	1.9	4
122	On-Surface Assembly of Hydrogen- and Halogen-Bonded Supramolecular Graphyne-Like Networks. <i>Angewandte Chemie</i> , 2020, 132, 9636-9642.	2.0	3
123	Surface oxidation-induced restructuring of liquid Pd-Ga SCALMS model catalysts. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 16324-16333.	2.8	3
124	Topological Phase Transitions in Zinc-Blende Semimetals Driven Exclusively by Electronic Temperature. <i>Physical Review Letters</i> , 2018, 120, 146401.	7.8	2
125	Assessment of quality and reliability of band structures from exact-exchange-only Kohn-Sham, hybrid, and GW methods. <i>European Physical Journal B</i> , 2018, 91, 1.	1.5	2
126	Selektivitätskontrolle in elektrokatalytischen Oxidationsreaktionen durch Ionische Flüssigkeiten. <i>Angewandte Chemie</i> , 2022, 134, .	2.0	2



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127	Liebmann-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
128	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
129	Numerically stable inversion approach to construct Kohn-Sham potentials for given electron densities within a Gaussian basis set framework. Journal of Chemical Physics, 0, , .	3.0	1
130	Supraparticles for Bare Eye H <sub>2</sub> Indication and Monitoring: Design, Working Principle, and Molecular Mobility (Adv. Funct. Mater. 22/2022). Advanced Functional Materials, 2022, 32, .	14.9	1
131	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
132	Thin Films: Area-Selective Growth of HfS <sub>2</sub> Thin Films via Atomic Layer Deposition at Low Temperature (Adv. Mater. Interfaces 23/2020). Advanced Materials Interfaces, 2020, 7, 2070130.	3.7	0
133	An embedded atom model for Ga-Pd systems: From intermetallic crystals to liquid alloys. Journal of Chemical Physics, 2021, 154, 014109.	3.0	0