Erin Johnson

List of Publications by Year
in descending order

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139 papers	22,628 citations	50276 46 h-index	10734 138 g-index
152 all docs	152 docs citations	152 times ranked	18069 citing authors

#	Article	IF	Citations
1	Revealing Noncovalent Interactions. Journal of the American Chemical Society, 2010, 132, 6498-6506.	13.7	6,465
2	NCIPLOT: A Program for Plotting Noncovalent Interaction Regions. Journal of Chemical Theory and Computation, 2011, 7, 625-632.	5.3	2,897
3	Predicting the Activity of Phenolic Antioxidants:Â Theoretical Method, Analysis of Substituent Effects, and Application to Major Families of Antioxidants. Journal of the American Chemical Society, 2001, 123, 1173-1183.	13.7	1,367
4	A simple effective potential for exchange. Journal of Chemical Physics, 2006, 124, 221101.	3.0	1,200
5	A density-functional model of the dispersion interaction. Journal of Chemical Physics, 2005, 123, 154101.	3.0	1,150
6	A post-Hartree-Fock model of intermolecular interactions: Inclusion of higher-order corrections. Journal of Chemical Physics, 2006, 124, 174104.	3.0	896
7	A post-Hartreeâ€“Fock model of intermolecular interactions. Journal of Chemical Physics, 2005, 123, 024101.	3.0	735
8	Exchange-hole dipole moment and the dispersion interaction. Journal of Chemical Physics, 2005, 122, 154104.	3.0	497
9	Critic2: A program for real-space analysis of quantum chemical interactions in solids. Computer Physics Communications, 2014, 185, 1007-1018.	7.5	497
10	Exchange-hole dipole moment and the dispersion interaction revisited. Journal of Chemical Physics, 2007, 127, 154108.	3.0	432
11	Analysis of Hydrogen-Bond Interaction Potentials from the Electron Density: Integration of Noncovalent Interaction Regions. Journal of Physical Chemistry A, 2011, 115, 12983-12990.	2.5	339
12	Dispersion interactions in densityâ€functional theory. Journal of Physical Organic Chemistry, 2009, 22, 1127-1135.	1.9	322
13	A benchmark for non-covalent interactions in solids. Journal of Chemical Physics, 2012, 137, 054103.	3.0	300
14	Revealing non-covalent interactions in solids: NCI plots revisited. Physical Chemistry Chemical Physics, 2012, 14, 12165.	2.8	279
15	Application of 25 density functionals to dispersion-bound homomolecular dimers. Chemical Physics Letters, 2004, 394, 334-338.	2.6	237
16	Van der Waals interactions in solids using the exchange-hole dipole moment model. Journal of Chemical Physics, 2012, 136, 174109.	3.0	197
17	A unified density-functional treatment of dynamical, nondynamical, and dispersion correlations. Journal of Chemical Physics, 2007, 127, 124108.	3.0	193
18	Lone Pairâ^Ï€ and Ï€â^Ï€ Interactions Play an Important Role in Proton-Coupled Electron Transfer Reactions. Journal of the American Chemical Society, 2007, 129, 6199-6203.	13.7	185

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19	Exchange-hole dipole moment and the dispersion interaction: High-order dispersion coefficients. Journal of Chemical Physics, 2006, 124, 014104.	3.0	184
20	Delocalization errors in density functionals and implications for main-group thermochemistry. Journal of Chemical Physics, 2008, 129, 204112.	3.0	159
21	Naphthalene Diols:Â A New Class of Antioxidants Intramolecular Hydrogen Bonding in Catechols, Naphthalene Diols, and Their Aryloxyl Radicals. Journal of Organic Chemistry, 2002, 67, 5190-5196.	3.2	154
22	Oscillations in meta-generalized-gradient approximation potential energy surfaces for dispersion-bound complexes. Journal of Chemical Physics, 2009, 131, 034111.	3.0	153
23	Patterning of Vinylferrocene on Hâ^'Si(100) via Self-Directed Growth of Molecular Lines and STM-Induced Decomposition. Nano Letters, 2002, 2, 807-810.	9.1	139
24	Structure and binding energies in van der Waals dimers: Comparison between density functional theory and correlated ab initio methods. Chemical Physics Letters, 2006, 419, 333-339.	2.6	136
25	Emergent Properties of an Organic Semiconductor Driven by its Molecular Chirality. ACS Nano, 2017, 11, 8329-8338.	14.6	136
26	Non-covalent interactions and thermochemistry using XDM-corrected hybrid and range-separated hybrid density functionals. Journal of Chemical Physics, 2013, 138, 204109.	3.0	130
27	Performance of conventional and dispersion-corrected density-functional theory methods for hydrogen bonding interaction energies. Physical Chemistry Chemical Physics, 2013, 15, 12821.	2.8	120
28	Origin of Nanoscale Friction Contrast between Supported Graphene, MoS₂, and a Graphene/MoS₂ Heterostructure. Nano Letters, 2019, 19, 5496-5505.	9.1	115
29	Density Functional Theory Based Model Calculations for Accurate Bond Dissociation Enthalpies. 3. A Single Approach for Xâ^'H, Xâ^'X, and Xâ^'Y (X, Y = C, N, O, S, Halogen) Bonds. Journal of Physical Chemistry A, 2003, 107, 9953-9963.	2.5	109
30	Singletâ^'Triplet Energy Gaps for Diradicals from Fractional-Spin Density-Functional Theory. Journal of Physical Chemistry A, 2011, 115, 76-83.	2.5	107
31	Large negative thermal expansion of a polymer driven by a submolecular conformational change. Nature Chemistry, 2013, 5, 1035-1041.	13.6	103
32	Halogen Bonding from Dispersion-Corrected Density-Functional Theory: The Role of Delocalization Error. Journal of Chemical Theory and Computation, 2014, 10, 5436-5447.	5.3	100
33	Extreme density-driven delocalization error for a model solvated-electron system. Journal of Chemical Physics, 2013, 139, 184116.	3.0	93
34	Density-functional description of electrides. Physical Chemistry Chemical Physics, 2014, 16, 14584-14593.	2.8	76
35	Structure and formation of highly luminescent protein-stabilized gold clusters. Chemical Science, 2018, 9, 2782-2790.	7.4	76
36	Delocalization error of density-functional approximations: A distinct manifestation in hydrogen molecular chains. Journal of Chemical Physics, 2012, 137, 214106.	3.0	66

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37	Many-body dispersion interactions from the exchange-hole dipole moment model. Journal of Chemical Physics, 2013, 138, 054103.	3.0	65
38	Theoretical Descriptors of Electrides. Journal of Physical Chemistry A, 2018, 122, 9371-9391.	2.5	63
39	Van der Waals interactions from the exchange hole dipole moment: Application to bio-organic benchmark systems. Chemical Physics Letters, 2006, 432, 600-603.	2.6	61
40	Predicting the Relative Solubilities of Racemic and Enantiopure Crystals by Densityâ€Functional Theory. Angewandte Chemie - International Edition, 2014, 53, 7879-7882.	13.8	56
41	Exchange-Hole Dipole Dispersion Model for Accurate Energy Ranking in Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2017, 13, 441-450.	5.3	56
42	Density-functional errors in ionization potential with increasing system size. Journal of Chemical Physics, 2015, 142, 184106.	3.0	52
43	Bisphosphineâ€Ligated Nickel Preâ€catalysts in C(sp²)â€“N Crossâ€Couplings of Aryl Chlorides: A Comparison of Nickel(I) and Nickel(II). Advanced Synthesis and Catalysis, 2017, 359, 2972-2980.	4.3	51
44	Adsorption of Organic Molecules on Kaolinite from the Exchange-Hole Dipole Moment Dispersion Model. Journal of Chemical Theory and Computation, 2012, 8, 5124-5131.	5.3	50
45	A computational exploration of the crystal energy and charge-carrier mobility landscapes of the chiral [6]helicene molecule. Nanoscale, 2018, 10, 1865-1876.	5.6	48
46	Metallophilic interactions from dispersion-corrected density-functional theory. Journal of Chemical Physics, 2014, 140, 18A504.	3.0	47
47	Carbon Nanotube Chirality Determines Efficiency of Electron Transfer to Fullerene in All-Carbon Photovoltaics. Journal of Physical Chemistry Letters, 2013, 4, 2914-2918.	4.6	46
48	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acidâ€“Base Coâ€Crystals. Angewandte Chemie - International Edition, 2018, 57, 14906-14910.	13.8	45
49	Hydroboration Catalyzed by 1,2,4,3-Triazaphospholenes. Organic Letters, 2017, 19, 5565-5568.	4.6	44
50	Surface Adsorption from the Exchange-Hole Dipole Moment Dispersion Model. Journal of Chemical Theory and Computation, 2016, 12, 3305-3315.	5.3	43
51	Delocalization error: The greatest outstanding challenge in densityâ€functional theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	14.6	43
52	Efficient silicon surface and cluster modeling using quantum capping potentials. Journal of Chemical Physics, 2005, 122, 044708.	3.0	42
53	Communication: DFT treatment of strong correlation in 3d transition-metal diatomics. Journal of Chemical Physics, 2017, 146, 211105.	3.0	42
54	Modeling Noncovalent Radicalâ€“Molecule Interactions Using Conventional Density-Functional Theory: Beware Erroneous Charge Transfer. Journal of Physical Chemistry A, 2013, 117, 947-952.	2.5	41

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55	Evaluating Force-Field London Dispersion Coefficients Using the Exchange-Hole Dipole Moment Model. Journal of Chemical Theory and Computation, 2017, 13, 6146-6157.	5.3	40
56	A unified density-functional treatment of dynamical, nondynamical, and dispersion correlations. II. Thermochemical and kinetic benchmarks. Journal of Chemical Physics, 2008, 128, 124105.	3.0	39
57	Predicting Energetics of Supramolecular Systems Using the XDM Dispersion Model. Journal of Chemical Theory and Computation, 2015, 11, 4033-4040.	5.3	39
58	Requirements for an accurate dispersion-corrected density functional. Journal of Chemical Physics, 2021, 154, 230902.	3.0	39
59	Local-hybrid functional based on the correlation length. Journal of Chemical Physics, 2014, 141, 124120.	3.0	38
60	The Exchange-Hole Dipole Moment Dispersion Model. , 2017, , 169-194.		37
61	(Ag,Cu)â€“Taâ€“O Ternaries As High-Temperature Solid-Lubricant Coatings. ACS Applied Materials & Interfaces, 2015, 7, 15422-15429.	8.0	32
62	Evaluating the London Dispersion Coefficients of Protein Force Fields Using the Exchange-Hole Dipole Moment Model. Journal of Physical Chemistry B, 2018, 122, 6690-6701.	2.6	32
63	Dependence of dispersion coefficients on atomic environment. Journal of Chemical Physics, 2011, 135, 234109.	3.0	31
64	Communication: A density functional with accurate fractional-charge and fractional-spin behaviour for s-electrons. Journal of Chemical Physics, 2011, 135, 081103.	3.0	31
65	Exchange-Hole Dipole Dispersion Model for Accurate Energy Ranking in Molecular Crystal Structure Prediction II: Nonplanar Molecules. Journal of Chemical Theory and Computation, 2017, 13, 5332-5342.	5.3	31
66	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. Journal of Computational Chemistry, 2020, 41, 427-438.	3.3	31
67	Effect of tip shape on atomic-friction at graphite step edges. Applied Physics Letters, 2013, 103, 081601.	3.3	30
68	What is â€œmany-bodyâ€•dispersion and should I worry about it?. Physical Chemistry Chemical Physics, 2020, 22, 8266-8276.	2.8	30
69	Density functionals and transition-metal atoms. Journal of Chemical Physics, 2007, 126, 184104.	3.0	29
70	Efficient basis sets for non-covalent interactions in XDM-corrected density-functional theory. Journal of Chemical Physics, 2013, 139, 214109.	3.0	29
71	Reevaluating the Stability and Prevalence of Conglomerates: Implications for Preferential Crystallization. Crystal Growth and Design, 2016, 16, 6055-6059.	3.0	29
72	Variational fractional-spin density-functional theory for diradicals. Journal of Chemical Physics, 2012, 137, 114112.	3.0	27

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73	Application of Diazaphospholidine/Diazaphospholene-Based Bisphosphines in Room-Temperature Nickel-Catalyzed C(sp²)â€“N Cross-Couplings of Primary Alkylamines with (Hetero)aryl Chlorides and Bromides. ACS Catalysis, 2018, 8, 5328-5339.	11.2	26
74	Theoretical Study of Dispersion Binding of Hydrocarbon Molecules to Hydrogen-Terminated Silicon(100)-2Ã—1. Journal of Physical Chemistry C, 2009, 113, 5681-5689.	3.1	24
75	Tests of an exact-exchange-based density-functional theory on transition-metal complexes. Canadian Journal of Chemistry, 2009, 87, 1369-1373.	1.1	24
76	Exchangeâ€“Correlation Effects for Noncovalent Interactions in Density Functional Theory. Journal of Chemical Theory and Computation, 2016, 12, 3160-3175.	5.3	24
77	Balancing Exchange Mixing in Density-Functional Approximations for Iron Porphyrin. Journal of Chemical Theory and Computation, 2015, 11, 3022-3028.	5.3	22
78	Adsorption of graphene to metal (111) surfaces using the exchange-hole dipole moment model. Carbon, 2017, 124, 531-540.	10.3	22
79	Dispersion XDM with Hybrid Functionals: Delocalization Error and Halogen Bonding in Molecular Crystals. Journal of Chemical Theory and Computation, 2019, 15, 4933-4944.	5.3	22
80	Communication: Correct charge transfer in CT complexes from the Beckeâ€™05 density functional. Journal of Chemical Physics, 2018, 148, 211101.	3.0	20
81	Chemical Basis of the Tribological Properties of AgTaO₃ Crystal Surfaces. Journal of Physical Chemistry C, 2014, 118, 17577-17584.	3.1	18
82	Oscillatory motion in layered materials: graphene, boron nitride, and molybdenum disulfide. Nanotechnology, 2015, 26, 165701.	2.6	18
83	Adsorption of graphene to nickel (111) using the exchange-hole dipole moment model. Carbon, 2017, 118, 184-191.	10.3	18
84	Composite and Low-Cost Approaches for Molecular Crystal Structure Prediction. Journal of Chemical Theory and Computation, 2018, 14, 2265-2276.	5.3	18
85	Evaluation of Shear-Slip Transitions in Crystalline Aspirin by Density-Functional Theory. Crystal Growth and Design, 2016, 16, 6867-6873.	3.0	17
86	Asymptotic Pairwise Dispersion Corrections Can Describe Layered Materials Accurately. Journal of Physical Chemistry Letters, 2020, 11, 2298-2302.	4.6	17
87	Convergence of calculated nuclear magnetic resonance chemical shifts in a protein with respect to quantum mechanical model size. Computational and Theoretical Chemistry, 2009, 898, 56-61.	1.5	16
88	Density-Functional Errors in Alkanes: A Real-Space Perspective. Journal of Chemical Theory and Computation, 2012, 8, 2676-2681.	5.3	16
89	The explicit examination of the magnetic states of electrides. Physical Chemistry Chemical Physics, 2016, 18, 27326-27335.	2.8	16
90	The ionic versus metallic nature of 2D electrides: a density-functional description. Physical Chemistry Chemical Physics, 2017, 19, 27343-27352.	2.8	16

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91	Radicals as hydrogen bond donors and acceptors. Interdisciplinary Sciences, Computational Life Sciences, 2009, 1, 133-140.	3.6	15
92	A density functional for strong correlation in atoms. Journal of Chemical Physics, 2013, 139, 074110.	3.0	15
93	Interrogating the Beckeâ€™05 density functional for non-locality information. Journal of Chemical Physics, 2017, 147, 154103.	3.0	15
94	Are dispersion corrections accurate outside equilibrium? A case study on benzene. Beilstein Journal of Organic Chemistry, 2018, 14, 1181-1191.	2.2	15
95	Spin-state splittings, highest-occupied-molecular-orbital and lowest-unoccupied-molecular-orbital energies, and chemical hardness. Journal of Chemical Physics, 2010, 133, 164107.	3.0	14
96	Chemical bonding and surface interactions in Bi2Se3 and Bi4Se3. Computational and Theoretical Chemistry, 2015, 1053, 238-244.	2.5	14
97	Pressure-Induced Isostructural Antiferromagneticâ€“Ferromagnetic Transition in an Organic Electride. Journal of Physical Chemistry C, 2018, 122, 12742-12747.	3.1	14
98	Crystal-energy landscapes of active pharmaceutical ingredients using composite approaches. CrystEngComm, 2019, 21, 5995-6009.	2.6	14
99	Theoretical modeling of structural superlubricity in rotated bilayer graphene, hexagonal boron nitride, molybdenum disulfide, and blue phosphorene. Nanoscale, 2021, 13, 14399-14407.	5.6	13
100	Hydrogen-bond strengths in large complexes: Efficient calculations using locally dense basis sets. Chemical Physics Letters, 2007, 435, 201-207.	2.6	12
101	Pentacene Binds Strongly to Hydrogen-Terminated Silicon Surfaces Via Dispersion Interactions. Journal of Physical Chemistry C, 2009, 113, 9969-9973.	3.1	12
102	An empirical model for silver tantalate. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 055002.	2.0	12
103	Quantitative Electron Delocalization in Solids from Maximally Localized Wannier Functions. Journal of Chemical Theory and Computation, 2018, 14, 4699-4710.	5.3	12
104	Gold(<scp>i</scp>) sulfide: unusual bonding and an unexpected computational challenge in a simple solid. Chemical Science, 2019, 10, 6467-6475.	7.4	12
105	Counterintuitive electron localisation from density-functional theory with polarisable solvent models. Journal of Chemical Physics, 2015, 143, 184112.	3.0	11
106	Application of XDM to ionic solids: The importance of dispersion for bulk moduli and crystal geometries. Journal of Chemical Physics, 2020, 153, 054121.	3.0	11
107	Computational Screening of Chiral Organic Semiconductors: Exploring Side-Group Functionalization and Assembly to Optimize Charge Transport. Crystal Growth and Design, 2021, 21, 5036-5049.	3.0	11
108	Reply to comment on â€˜Application of 25 density functionals to dispersion-bound homomolecular dimersâ€™ [Chem. Phys. Lett. 394 (2004) 334â€“338]. Chemical Physics Letters, 2005, 401, 595-596.	2.6	10

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109	Judging Density-Functional Approximations: Some Pitfalls of Statistics. Topics in Current Chemistry, 2014, , 81-95.	4.0	10
110	Pervasive Delocalisation Error Causes Spurious Proton Transfer in Organic Acidâ€“Base Coâ€€Crystals. Angewandte Chemie, 2018, 130, 15122-15126.	2.0	10
111	Probing the Influence of PAd-DalPhos Ancillary Ligand Structure on Nickel-Catalyzed Ammonia Cross-Coupling. Organometallics, 2018, 37, 4015-4023.	2.3	10
112	Identification of a Nitrenoid Reductive Elimination Pathway in Nickel-Catalyzed Câ€“N Cross-Coupling. ACS Catalysis, 2022, 12, 1475-1480.	11.2	10
113	Contributions of pauli repulsions to the energetics and physical properties computed in QM/MM methods. Journal of Computational Chemistry, 2013, 34, 2380-2388.	3.3	9
114	Effect of a Metal Substrate on Interlayer Interactions in Bilayer Graphene. Journal of Physical Chemistry C, 2018, 122, 8910-8918.	3.1	9
115	Density-functional description of alkalides: introducing the alkalide state. Physical Chemistry Chemical Physics, 2018, 20, 26710-26718.	2.8	9
116	Communication: Beckeâ€™s virial exciton model gives accurate charge-transfer excitation energies. Journal of Chemical Physics, 2018, 149, 231101.	3.0	9
117	Non-Covalent Interactions in Molecular Crystals: Exploring the Accuracy of the Exchange-Hole Dipole Moment Model with Local Orbitals. Journal of Chemical Theory and Computation, 2018, 14, 5715-5724.	5.3	9
118	The effect of electronic excitation on London dispersion. Canadian Journal of Chemistry, 2018, 96, 730-737.	1.1	9
119	Theoretical investigation of polymorph- and coformer-dependent photoluminescence in molecular crystals. CrystEngComm, 2021, 23, 4264-4271.	2.6	9
120	Clusters in Liquid Fatty Acids: Structure and Role in Nucleation. Journal of Physical Chemistry B, 2019, 123, 7043-7054.	2.6	8
121	Hydrostibination of Alkynes: A Radical Mechanism**. Chemistry - A European Journal, 2020, 26, 17134-17142.	3.3	8
122	The Relative Thermodynamic Stability of Diamond and Graphite. Angewandte Chemie - International Edition, 2021, 60, 1546-1549.	13.8	8
123	Thermodynamic cycles of the alkali metalâ€“ligand complexes central to electride formation. Physical Chemistry Chemical Physics, 2017, 19, 12816-12825.	2.8	7
124	Theoretical investigation of amino-acid adsorption on hydroxylated quartz surfaces: dispersion can determine enantioselectivity. Physical Chemistry Chemical Physics, 2020, 22, 16571-16578.	2.8	7
125	A density-functional benchmark of vibrational free-energy corrections for molecular crystal polymorphism. Journal of Chemical Physics, 2022, 156, 114108.	3.0	7
126	New XDM-corrected potential energy surfaces for Arâ€“NO(X2Î): A comparison with CCSD(T) calculations and experiments. Journal of Chemical Physics, 2015, 142, 024302.	3.0	6

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127	Potent Inhibition of Mandelate Racemase by Boronic Acids: Boron as a Mimic of a Carbon Acid Center. Biochemistry, 2020, 59, 3026-3037.	2.5	6
128	Kinetics of the Addition of Olefins to Si-Centered Radicals: The Critical Role of Dispersion Interactions Revealed by Theory and Experiment. Journal of Physical Chemistry A, 2015, 119, 5883-5888.	2.5	5
129	Analysis of Density-Functional Errors for Noncovalent Interactions between Charged Molecules. Journal of Physical Chemistry A, 2020, 124, 353-361.	2.5	5
130	Improved Charge Transfer and Barrier Lowering across a Auâ€“MoS₂ Interface through Insertion of a Layered Ca₂N Electride. Journal of Physical Chemistry C, 2021, 125, 11656-11664.	3.1	5
131	Computational modeling of piezochromism in molecular crystals. Journal of Chemical Physics, 2020, 152, 234106.	3.0	4
132	Improved quantitative crystal-structure comparison using powder diffractograms via anisotropic volume correction. CrystEngComm, 2021, 23, 7118-7131.	2.6	4
133	Interplay between London Dispersion, Hubbard U, and Metastable States for Uranium Compounds. Journal of Physical Chemistry A, 2021, 125, 2791-2799.	2.5	4
134	The role of roughness-induced damping in the oscillatory motion of bilayer graphene. Nanotechnology, 2014, 25, 425703.	2.6	2
135	Directed Ortho and Remote Metalation of Naphthalene 1,8-Diamide: Complementing S_EAr Reactivity for the Synthesis of Substituted Naphthalenes. Organic Letters, 2021, 23, 1966-1973.	4.6	2
136	Noncovalent Interactions in Organic Radicals: Pancake, Ïƒ-Hole, and H-Bonding in F2HbimDTDA. Crystal Growth and Design, 0, , .	3.0	2
137	van der Waals potential energy surfaces from the exchange-hole dipole moment dispersion model. Canadian Journal of Chemistry, 2016, 94, 1049-1056.	1.1	1
138	Density Functional Theory Based Model Calculations for Accurate Bond Dissociation Enthalpies. Part 3. A Single Approach for Xâ€”H, Xâ€”X, and Xâ€”Y, (X, Y: C, N, O, S, Halogen) Bonds.. ChemInform, 2004, 35, no.	0.0	0
139	The Relative Thermodynamic Stability of Diamond and Graphite. Angewandte Chemie, 2021, 133, 1570-1573.	2.0	0