Stefan Goedecker

List of Publications by Year
in descending order

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148 papers	21,613 citations	31902 53 h-index	8835 145 g-index
151 all docs	151 docs citations	151 times ranked	17455 citing authors

#	Article	IF	Citations
1	Separable dual-space Gaussian pseudopotentials. Physical Review B, 1996, 54, 1703-1710.	1.1	5,153
2	Relativistic separable dual-space Gaussian pseudopotentials from H to Rn. Physical Review B, 1998, 58, 3641-3662.	1.1	3,201
3	ABINIT: First-principles approach to material and nanosystem properties. Computer Physics Communications, 2009, 180, 2582-2615.	3.0	2,297
4	Linear scaling electronic structure methods. Reviews of Modern Physics, 1999, 71, 1085-1123.	16.4	1,247
5	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	6.0	1,113
6	Minima hopping: An efficient search method for the global minimum of the potential energy surface of complex molecular systems. Journal of Chemical Physics, 2004, 120, 9911-9917.	1.2	697
7	Efficient Linear Scaling Algorithm for Tight-Binding Molecular Dynamics. Physical Review Letters, 1994, 73, 122-125.	2.9	412
8	Crystal Structure of Cold Compressed Graphite. Physical Review Letters, 2012, 108, 065501.	2.9	292
9	Daubechies wavelets as a basis set for density functional pseudopotential calculations. Journal of Chemical Physics, 2008, 129, 014109.	1.2	289
10	Crystal structure prediction using the minima hopping method. Journal of Chemical Physics, 2010, 133, 224104.	1.2	253
11	Natural Orbital Functional for the Many-Electron Problem. Physical Review Letters, 1998, 81, 866-869.	2.9	224
12	A fourth-generation high-dimensional neural network potential with accurate electrostatics including non-local charge transfer. Nature Communications, 2021, 12, 398.	5.8	215
13	Fast Radix 2, 3, 4, and 5 Kernels for Fast Fourier Transformations on Computers with Overlapping Multiply–Add Instructions. SIAM Journal of Scientific Computing, 1997, 18, 1605-1611.	1.3	195
14	Tight-binding electronic-structure calculations and tight-binding molecular dynamics with localized orbitals. Physical Review B, 1995, 51, 9455-9464.	1.1	181
15	Interatomic potentials for ionic systems with density functional accuracy based on charge densities obtained by a neural network. Physical Review B, 2015, 92, .	1.1	179
16	Energy Landscape of Fullerene Materials: A Comparison of Boron to Boron Nitride and Carbon. Physical Review Letters, 2011, 106, 225502.	2.9	169
17	Ultralow Thermal Conductivity in Full Heusler Semiconductors. Physical Review Letters, 2016, 117, 046602.	2.9	163
18	Accurate and efficient linear scaling DFT calculations with universal applicability. Physical Chemistry Chemical Physics, 2015, 17, 31360-31370.	1.3	158

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19	Critical assessment of the self-interaction-correctedâ€“local-density-functional method and its algorithmic implementation. Physical Review A, 1997, 55, 1765-1771.	1.0	155
20	Decay properties of the finite-temperature density matrix in metals. Physical Review B, 1998, 58, 3501-3502.	1.1	147
21	Daubechies wavelets for linear scaling density functional theory. Journal of Chemical Physics, 2014, 140, 204110.	1.2	140
22	Low-energy silicon allotropes with strong absorption in the visible for photovoltaic applications. Physical Review B, 2012, 86, .	1.1	138
23	Global Minimum Determination of the Born-Oppenheimer Surface within Density Functional Theory. Physical Review Letters, 2005, 95, 055501.	2.9	136
24	Low Complexity Algorithms for Electronic Structure Calculations. Journal of Computational Physics, 1995, 118, 261-268.	1.9	127
25	Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure. Physical Review B, 2016, 93, .	1.1	125
26	Extended Halogen Bonding between Fully Fluorinated Aromatic Molecules. ACS Nano, 2015, 9, 2574-2583.	7.3	119
27	Metrics for measuring distances in configuration spaces. Journal of Chemical Physics, 2013, 139, 184118.	1.2	116
28	Transferability of pseudopotentials. Physical Review A, 1992, 45, 88-93.	1.0	113
29	A Fourfold Coordinated Point Defect in Silicon. Physical Review Letters, 2002, 88, 235501.	2.9	102
30	Norm-conserving pseudopotentials with chemical accuracy compared to all-electron calculations. Journal of Chemical Physics, 2013, 138, 104109.	1.2	95
31	Chemical Wiring and Soldering toward All-Molecule Electronic Circuitry. Journal of the American Chemical Society, 2011, 133, 8227-8233.	6.6	93
32	A fingerprint based metric for measuring similarities of crystalline structures. Journal of Chemical Physics, 2016, 144, 034203.	1.2	93
33	A generalized Poisson and Poisson-Boltzmann solver for electrostatic environments. Journal of Chemical Physics, 2016, 144, 014103.	1.2	88
34	The Elephant in the Room of Density Functional Theory Calculations. Journal of Physical Chemistry Letters, 2017, 8, 1449-1457.	2.1	88
35	High-Pressure Structures of Disilane and Their Superconducting Properties. Physical Review Letters, 2012, 108, 117004.	2.9	86
36	The performance of minima hopping and evolutionary algorithms for cluster structure prediction. Journal of Chemical Physics, 2009, 130, 144108.	1.2	83

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37	Soft-Sphere Continuum Solvation in Electronic-Structure Calculations. Journal of Chemical Theory and Computation, 2017, 13, 3829-3845.	2.3	76
38	Low-density silicon allotropes for photovoltaic applications. Physical Review B, 2015, 92, .	1.1	70
39	Two-Dimensional Hexagonal Sheet of TiO₂. Chemistry of Materials, 2017, 29, 8594-8603.	3.2	69
40	High accuracy and transferability of a neural network potential through charge equilibration for calcium fluoride. Physical Review B, 2017, 95, .	1.1	68
41	Bell-Evans-Polanyi principle for molecular dynamics trajectories and its implications for global optimization. Physical Review E, 2008, 77, 056707.	0.8	67
42	Efficient moves for global geometry optimization methods and their application to binary systems. Journal of Chemical Physics, 2011, 134, 044106.	1.2	65
43	General-Purpose Machine Learning Potentials Capturing Nonlocal Charge Transfer. Accounts of Chemical Research, 2021, 54, 808-817.	7.6	65
44	Questioning the existence of a unique ground-state structure for Si clusters. Physical Review B, 2007, 75, .	1.1	62
45	Structure of large gold clusters obtained by global optimization using the minima hopping method. Physical Review B, 2009, 79, .	1.1	62
46	Linear scaling solution of the Coulomb problem using wavelets. Solid State Communications, 1998, 105, 665-669.	0.9	61
47	Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194110.	1.2	60
48	Structure and stability of semiconductor tip apexes for atomic force microscopy. Nanotechnology, 2009, 20, 264015.	1.3	59
49	Multiscale approach for simulations of Kelvin probe force microscopy with atomic resolution. Physical Review B, 2012, 86, .	1.1	59
50	Quantifying the atomic-level mechanics of single long physisorbed molecular chains. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 3968-3972.	3.3	59
51	Sodiumâ€“gold binaries: novel structures for ionic compounds from anab initiostructural search. New Journal of Physics, 2013, 15, 115007.	1.2	58
52	Tight-Binding Molecular Dynamics of Shock Waves in Methane. Physical Review Letters, 1999, 83, 3896-3899.	2.9	57
53	Obtaining Detailed Structural Information about Supramolecular Systems on Surfaces by Combining High-Resolution Force Microscopy with ab Initio Calculations. ACS Nano, 2013, 7, 9098-9105.	7.3	56
54	Identification of Novel Cu, Ag, and Au Ternary Oxides from Global Structural Prediction. Chemistry of Materials, 2015, 27, 4562-4573.	3.2	56

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55	Precise engineering of quantum dot array coupling through their barrier widths. Nature Communications, 2017, 8, 787.	5.8	55
56	Ubiquitous Mechanisms of Energy Dissipation in Noncontact Atomic Force Microscopy. Physical Review Letters, 2008, 100, 236106.	2.9	53
57	Daubechies wavelets for high performance electronic structure calculations: The BigDFT project. Comptes Rendus - Mecanique, 2011, 339, 149-164.	2.1	53
58	Growth and Structural Properties of Mg_N (N = 10â€“56) Clusters: Density Functional Theory Study. Journal of Physical Chemistry A, 2011, 115, 12307-12314.	1.1	52
59	Organometallic Bonding in an Ullmann-Type On-Surface Chemical Reaction Studied by High-Resolution Atomic Force Microscopy. Small, 2016, 12, 5303-5311.	5.2	52
60	Integral representation of the Fermi distribution and its applications in electronic-structure calculations. Physical Review B, 1993, 48, 17573-17575.	1.1	49
61	Interplay between structure and superconductivity: Metastable phases of phosphorus under pressure. Physical Review Materials, 2017, 1, .	0.9	48
62	Discovery of a Superconducting Cuâ€“Bi Intermetallic Compound by Highâ€Pressure Synthesis. Angewandte Chemie - International Edition, 2016, 55, 13446-13449.	7.2	46
63	Novel Structural Motifs in Low Energy Phases of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>LiAlH</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2012, 108, 205505.	2.9	43
64	Solvent-Aware Interfaces in Continuum Solvation. Journal of Chemical Theory and Computation, 2019, 15, 1996-2009.	2.3	43
65	Isomerism and Structural Fluxionality in the Au₂₆ and Au₂₆^{â€“} Nanoclusters. ACS Nano, 2014, 8, 7413-7422.	7.3	42
66	Operator approach in the linearized augmented-plane-wave method: Efficient electronic-structure calculations including forces. Physical Review B, 1992, 45, 1597-1604.	1.1	40
67	Conducting Boron Sheets Formed by the Reconstruction of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-Boron (111) Surface. Physical Review Letters, 2013, 111, 136101.	2.9	40
68	Structural metastability of endohedral silicon fullerenes. Physical Review B, 2010, 81, .	1.1	39
69	Low-Energy Polymeric Phases of Alanates. Physical Review Letters, 2013, 110, 135502.	2.9	38
70	Minima hopping guided path search: An efficient method for finding complex chemical reaction pathways. Journal of Chemical Physics, 2014, 140, 214102.	1.2	38
71	A Minima Hopping Study of All-Atom Protein Folding and Structure Prediction. Journal of Physical Chemistry B, 2009, 113, 7315-7321.	1.2	37
72	Low-energy boron fullerenes: Role of disorder and potential synthesis pathways. Physical Review B, 2011, 83, .	1.1	37

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73	An assessment of the structural resolution of various fingerprints commonly used in machine learning. Machine Learning: Science and Technology, 2021, 2, 015018.	2.4	37
74	Rotating a three-dimensional array in an optimal position for vector processing: case study for a three-dimensional fast Fourier transform. Computer Physics Communications, 1993, 76, 294-300.	3.0	35
75	Solution of Multiscale Partial Differential Equations Using Wavelets. Computers in Physics, 1998, 12, 548.	0.6	35
76	Computational acceleration of prospective dopant discovery in cuprous iodide. Physical Chemistry Chemical Physics, 2019, 21, 18839-18849.	1.3	34
77	Carbon structures and defect planes in diamond at high pressure. Physical Review B, 2013, 88, .	1.1	32
78	Energy landscape of silicon systems and its description by force fields, tight binding schemes, density functional methods, and quantum Monte Carlo methods. Physical Review B, 2010, 81, .	1.1	31
79	Frequency localization properties of the density matrix and its resulting hypersparsity in a wavelet representation. Physical Review B, 1999, 59, 7270-7273.	1.1	30
80	Thermodynamic stability of alkali-metalâ€“zinc double-cation borohydrides at low temperatures. Physical Review B, 2013, 88, .	1.1	29
81	Raman activity of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>s</mml:mi><mml:msup><mml:mi>p</mml:mi><mml:mn>3</mml:mn></mml:msup></mml:m allotropes under pressure: A density functional theory study. Physical Review B, 2012, 85, .	1.1	28
82	Characterization of individual molecular adsorption geometries by atomic force microscopy: Cu-TCPP on rutile TiO2 (110). Journal of Chemical Physics, 2015, 143, 094202.	1.2	28
83	Remark on Algorithms to Find Roots of Polynomials. SIAM Journal of Scientific Computing, 1994, 15, 1059-1063.	1.3	27
84	Low-energy structures of zinc borohydride Zn(BH<mml:math) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 317 Td (xmlns:mml="http://www.w3 xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	1.1	27
85	Relation between the Dynamics of Glassy Clusters and Characteristic Features of their Energy Landscape. Physical Review Letters, 2014, 112, .	2.9	27
86	Stable structures of exohedrally decorated C60-fullerenes. Carbon, 2018, 129, 847-853.	5.4	27
87	An efficient numerical quadrature for the calculation of the potential energy of wavefunctions expressed in the Daubechies wavelet basis. Journal of Computational Physics, 2006, 217, 312-339.	1.9	26
88	The effect of ionization on the global minima of small and medium sized silicon and magnesium clusters. Journal of Chemical Physics, 2011, 134, 124302.	1.2	25
89	First-principles predicted low-energy structures of NaSc(BH4)4. Journal of Chemical Physics, 2014, 140, 124708.	1.2	25
90	Rare-earth magnetic nitride perovskites. JPhys Materials, 2019, 2, 025003.	1.8	25

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91	Wet Environment Effects for Ethanol and Water Adsorption on Anatase TiO₂ (101) Surfaces. Journal of Physical Chemistry C, 2020, 124, 2406-2419.	1.5	24
92	Stabilized quasi-Newton optimization of noisy potential energy surfaces. Journal of Chemical Physics, 2015, 142, 034112.	1.2	23
93	Hydroxyl-Induced Partial Charge States of Single Porphyrins on Titania Rutile. Journal of Physical Chemistry C, 2017, 121, 3607-3614.	1.5	23
94	Emergence of superconductivity in doped H2O ice at high pressure. Scientific Reports, 2017, 7, 6825.	1.6	23
95	Locality properties and Wannier functions for interacting systems. Solid State Communications, 2001, 119, 105-109.	0.9	21
96	Novel crystal structures for lithiumâ€“silicon alloy predicted by minima hopping method. Journal of Alloys and Compounds, 2016, 655, 147-154.	2.8	21
97	Missing theoretical evidence for conventional room-temperature superconductivity in low-enthalpy structures of carbonaceous sulfur hydrides. Physical Review Materials, 2022, 6, .	0.9	20
98	Evidence for carbon clusters present near thermal gate oxides affecting the electronic band structure in SiC-MOSFET. Applied Physics Letters, 2019, 115, .	1.5	19
99	Surfactant-assisted synthesis of large Cu-BTC MOF single crystals and their potential utilization as photodetectors. CrystEngComm, 2019, 21, 3948-3953.	1.3	19
100	Alternative approach to separable first-principles pseudopotentials. Physical Review B, 1990, 42, 8858-8863.	1.1	18
101	Optimization and parallelization of a force field for silicon using OpenMP. Computer Physics Communications, 2002, 148, 124-135.	3.0	18
102	An efficient 3-dim FFT for plane wave electronic structure calculations on massively parallel machines composed ofÂmultiprocessor nodes. Computer Physics Communications, 2003, 154, 105-110.	3.0	17
103	Surface reconstructions and premelting of the (100) CaF₂surface. Physical Chemistry Chemical Physics, 2019, 21, 16270-16281.	1.3	17
104	An enhanced splined saddle method. Journal of Chemical Physics, 2011, 135, 014108.	1.2	16
105	ZnSb Polymorphs with Improved Thermoelectric Properties. Chemistry of Materials, 2016, 28, 2912-2920.	3.2	16
106	Affordable and accurate large-scale hybrid-functional calculations on GPU-accelerated supercomputers. Journal of Physics Condensed Matter, 2018, 30, 095901.	0.7	16
107	A particle-particle, particle-density algorithm for the calculation of electrostatic interactions of particles with slablike geometry. Journal of Chemical Physics, 2007, 127, 224102.	1.2	15
108	Metastable exohedrally decorated Borospherene B40. Scientific Reports, 2017, 7, 7618.	1.6	15

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109	New Route for â€œCold-Passivationâ€•of Defects in Tin-Based Oxides. Journal of Physical Chemistry C, 2018, 122, 17612-17620.	1.5	15
110	Surface reconstruction of fluorites in vacuum and aqueous environment. Physical Review Materials, 2017, 1, .	0.9	15
111	Emergence of hidden phases of methylammonium lead iodide <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:msub><mml:mi>CH</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi>NH</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mo>)</mml:mo><mml:msub><mml:mi>PbI</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> upon compression. Physical Review Materials, 2018, 2, .	1.5	15
112	Manifolds of quasi-constant SOAP and ACSF fingerprints and the resulting failure to machine learn four-body interactions. Journal of Chemical Physics, 2022, 156, 034302.	1.2	15
113	Energy landscape of silicon tetraâ€•interstitials using an optimized classical potential. Physica Status Solidi (B): Basic Research, 2011, 248, 2050-2055.	0.7	14
114	Novel phases of lithium-aluminum binaries from first-principles structural search. Journal of Chemical Physics, 2015, 142, 024710.	1.2	14
115	Discovery of a Superconducting Cuâ€“Bi Intermetallic Compound by Highâ€Pressure Synthesis. Angewandte Chemie, 2016, 128, 13644-13647.	1.6	14
116	Prediction of a novel monoclinic carbon allotrope. European Physical Journal B, 2013, 86, 1.	0.6	13
117	The crystal structure of p-type transparent conductive oxide CuBO2. MRS Communications, 2013, 3, 157-160.	0.8	12
118	Computational Screening of Useful Holeâ€“Electron Dopants in SnO₂. Chemistry of Materials, 2017, 29, 10095-10103.	3.2	12
119	Atomic Friction: Anisotropy and Asymmetry Effects. Tribology Letters, 2019, 67, 1.	1.2	12
120	Nonexistence of the decahedral <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Si</mml:mi></mml:mrow><mml:mn>20</mml:mn></mml:msub></mml:math> cage: Levinthal's paradox revisited. Physical Review B, 2020, 101, .	1.1	12
121	Adsorption of small NaCl clusters on surfaces of silicon nanostructures. Nanotechnology, 2009, 20, 445301.	1.3	11
122	A customized 3D GPU Poisson solver for free boundary conditions. Computer Physics Communications, 2013, 184, 1815-1820.	3.0	11
123	Boron aggregation in the ground states of boron-carbon fullerenes. Physical Review B, 2014, 89, .	1.1	11
124	Chain-like structure elements in Ni40Ta60 metallic glasses observed by scanning tunneling microscopy. Scientific Reports, 2015, 5, 13143.	1.6	10
125	Computationally efficient characterization of potential energy surfaces based on fingerprint distances. Journal of Chemical Physics, 2016, 145, 034101.	1.2	10
126	Direct observation of single organic molecules grafted on the surface of a silicon nanowire. Scientific Reports, 2019, 9, 5647.	1.6	10

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127	Finding Reaction Pathways with Optimal Atomic Index Mappings. Physical Review Letters, 2019, 123, 206102.	2.9	10
128	Fingerprint-Based Detection of Non-Local Effects in the Electronic Structure of a Simple Single Component Covalent System. Condensed Matter, 2021, 6, 9.	0.8	10
129	Parallel O(N) tight-binding molecular dynamics of polyethylene and compressed methane. Journal of Computer-Aided Materials Design, 1998, 5, 295-316.	0.7	9
130	New strontium titanate polymorphs under high pressure. Journal of Computational Chemistry, 2021, 42, 699-705.	1.5	8
131	Funnel hopping Monte Carlo: An efficient method to overcome broken ergodicity. Journal of Chemical Physics, 2020, 152, 164106.	1.2	7
132	Controlled switching of a single CuPc molecule on Cu(111) at low temperature. Physical Review B, 2019, 100, .	1.1	6
133	Density functional investigations on structural and electronic properties of anionic and neutral sodium clusters Na_N(N= 40â€“147): comparison with the experimental photoelectron spectra. Journal of Physics Condensed Matter, 2011, 23, 405303.	0.7	5
134	Accelerated materials design approaches based on structural classification: application to low enthalpy high pressure phases of SH3 and SeH3. Novel Superconducting Materials, 2017, 3, .	0.8	5
135	Divalent Path to Enhance p-Type Conductivity in a SnO Transparent Semiconductor. Journal of Physical Chemistry C, 2019, 123, 14909-14913.	1.5	5
136	Large-scale structure prediction of near-stoichiometric magnesium oxide based on a machine-learned interatomic potential: Crystalline phases and oxygen-vacancy ordering. Physical Review Materials, 2021, 5, .	0.9	5
137	Comment on â€˜â€˜Criterion for a good variational wave functionâ€™â€™. Physical Review B, 1991, 44, 10365-10366.	3.6	4
138	Comment on â€œTopological Insulators in Ternary Compounds with a Honeycomb Latticeâ€• Physical Review Letters, 2013, 110, 129701.	2.9	4
139	Maximum volume simplex method for automatic selection and classification of atomic environments and environment descriptor compression. Journal of Chemical Physics, 2020, 153, 214104.	1.2	4
140	Energetic and vibrational analysis of hydrogenated silicon<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>m</mml:mi></mml:math>vacancies above saturation. Physical Review B, 2014, 90, .	1.1	3
141	Fast iterative diagonalization of nonlocal pseudopotential Hamiltonians using the fast Fourier transformation. Physical Review B, 1990, 41, 3230-3231.	1.1	2
142	Treatment of semicore states in the linearized augmented-plane-wave method and other linearized electronic-structure methods. Physical Review B, 1993, 47, 9881-9883.	1.1	2
143	Efficient iterative diagonalization of separable pseudopotential Hamiltonians. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1994, 70, 305-308.	0.6	2
144	Comment on â€œTowards Direct-Gap Silicon Phases by the Inverse Band Structure Design Approachâ€• Physical Review Letters, 2014, 112, 199801.	2.9	2

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145	Influence of an external electric field on the potential-energy surface of alkali-metal-decorated C60. Physical Review A, 2018, 97, .	1.0	2
146	Novel polymorphs and polytypes of lithium chloride from structure predictions based on charge equilibration via neural network technique. Physical Review Materials, 2021, 5, .	0.9	2
147	Linear scaling methods for the solution of schrÃ¶dinger's equation. Handbook of Numerical Analysis, 2003, 10, 537-570.	0.9	1
148	Connecting single conductive polymers to a single functional molecule. , 2010, , .		0