

# Ferdinand C Grozema

## List of Publications by Year in descending order

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118  
papers

7,038  
citations

53660

45  
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60497

81  
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119  
all docs

119  
docs citations

119  
times ranked

8586  
citing authors

#	ARTICLE	IF	CITATIONS
1	Towards high charge-carrier mobilities by rational design of the shape and periphery of discotics. <i>Nature Materials</i> , 2009, 8, 421-426.	13.3	555
2	Charge transport in columnar stacked triphenylenes: Effects of conformational fluctuations on charge transfer integrals and site energies. <i>Journal of Chemical Physics</i> , 2003, 119, 9809-9817.	1.2	395
3	Absolute Rates of Hole Transfer in DNA. <i>Journal of the American Chemical Society</i> , 2005, 127, 14894-14903.	6.6	325
4	Mechanism of Charge Migration through DNA: A Molecular Wire Behavior, Single-Step Tunneling or Hopping?. <i>Journal of the American Chemical Society</i> , 2000, 122, 10903-10909.	6.6	211
5	Signatures of Quantum Interference Effects on Charge Transport Through a Single Benzene Ring. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 3152-3155.	7.2	204
6	Mechanism of charge transport in self-organizing organic materials. <i>International Reviews in Physical Chemistry</i> , 2008, 27, 87-138.	0.9	194
7	Intramolecular Charge Transport along Isolated Chains of Conjugated Polymers: Effect of Torsional Disorder and Polymerization Defects. <i>Journal of Physical Chemistry B</i> , 2002, 106, 7791-7795.	1.2	186
8	High Intrachain Hole Mobility on Molecular Wires of Ladder-Type Poly(p-Phenylenes). <i>Physical Review Letters</i> , 2006, 96, 146601.	2.9	181
9	Hole Conduction along Molecular Wires: $\sigma$ -Bonded Silicon Versus $\pi$ -Bond-Conjugated Carbon. <i>Advanced Materials</i> , 2002, 14, 228-231.	11.1	167
10	Effect of Structural Dynamics on Charge Transfer in DNA Hairpins. <i>Journal of the American Chemical Society</i> , 2008, 130, 5157-5166.	6.6	148
11	Bimolecular Auger Recombination of Electron-Hole Pairs in Two-Dimensional CdSe and CdSe/CdZnS Core/Shell Nanoplatelets. <i>Journal of Physical Chemistry Letters</i> , 2013, 4, 3574-3578.	2.1	146
12	H-Bond-Stabilized Triphenylene-Based Columnar Discotic Liquid Crystals. <i>Chemistry of Materials</i> , 2006, 18, 968-974.	3.2	141
13	Temperature-Resolved Local and Macroscopic Charge Carrier Transport in Thin P3HT Layers. <i>Advanced Functional Materials</i> , 2010, 20, 2286-2295.	7.8	131
14	Charge Carrier Dynamics in Cs <sub>2</sub> AgBiBr <sub>6</sub> Double Perovskite. <i>Journal of Physical Chemistry C</i> , 2018, 122, 4809-4816.	1.5	131
15	Interconversion between Free Charges and Bound Excitons in 2D Hybrid Lead Halide Perovskites. <i>Journal of Physical Chemistry C</i> , 2017, 121, 26566-26574.	1.5	123
16	Nature and Decay Pathways of Photoexcited States in CdSe and CdSe/CdS Nanoplatelets. <i>Nano Letters</i> , 2014, 14, 7039-7045.	4.5	122
17	Radiative and Nonradiative Recombination in CuInS <sub>2</sub> Nanocrystals and CuInS <sub>2</sub> -Based Core/Shell Nanocrystals. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3503-3509.	2.1	119
18	Charge Transfer in Donor-Bridge-Acceptor Systems: Static Disorder, Dynamic Fluctuations, and Complex Kinetics. <i>Journal of Physical Chemistry C</i> , 2008, 112, 10988-11000.	1.5	114

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19	Hole Mobility in DNA: Effects of Static and Dynamic Structural Fluctuations. <i>ChemPhysChem</i> , 2002, 3, 536.	1.0	112
20	Mapping the Sites for Selective Oxidation of Guanines in DNA. <i>Journal of the American Chemical Society</i> , 2003, 125, 13658-13659.	6.6	97
21	Excited state polarizabilities of conjugated molecules calculated using time dependent density functional theory. <i>Journal of Chemical Physics</i> , 2001, 115, 10014-10021.	1.2	94
22	Supramolecular Control of Charge Transport in Molecular Wires. <i>Journal of the American Chemical Society</i> , 2007, 129, 13370-13371.	6.6	94
23	Charge Transport in Self-Organized $\pi$ -Stacks of <i>p</i> -Phenylene Vinylene Oligomers. <i>Journal of Physical Chemistry B</i> , 2005, 109, 18267-18274.	1.2	90
24	Biosupramolecular Nanowires from Chlorophyll Dyes with Exceptional Charge Transport Properties. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 6378-6382.	7.2	88
25	Density of Trap States and Auger-mediated Electron Trapping in CdTe Quantum-Dot Solids. <i>Nano Letters</i> , 2015, 15, 3056-3066.	4.5	84
26	Organic Linker Defines the Excited State Decay of Photocatalytic MIL-125(Ti)-Type Materials. <i>ChemSusChem</i> , 2016, 9, 388-395.	3.6	84
27	Band-Like Charge Transport in Cs <sub>2</sub> AgBiBr <sub>6</sub> and Mixed Antimony-Bismuth Cs <sub>2</sub> AgBi <sub>1-x</sub> Sb <sub>x</sub> Br <sub>6</sub> Halide Double Perovskites. <i>ACS Omega</i> , 2018, 3, 11655-11662.	1.6	84
28	Delocalization and Mobility of Charge Carriers in Covalent Organic Frameworks. <i>Journal of Physical Chemistry C</i> , 2011, 115, 11768-11772.	1.5	73
29	Quasi Temperature Independent Electron Mobility in Hexagonal Columnar Mesophases of an H-Bonded Benzotrithiophene Derivative. <i>Chemistry of Materials</i> , 2010, 22, 1420-1428.	3.2	72
30	Charge Mobilities in Conjugated Polymers Measured by Pulse Radiolysis Time-Resolved Microwave Conductivity: From Single Chains to Solids. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 2951-2958.	2.1	69
31	Theoretical and experimental studies of the opto-electronic properties of positively charged oligo(phenylene vinylene)s: Effects of chain length and alkoxy substitution. <i>Journal of Chemical Physics</i> , 2002, 117, 11366-11378.	1.2	65
32	Hydrogen-bond stabilized columnar discotic benzenetrisamides with pendant triphenylene groups. <i>Journal of Materials Chemistry</i> , 2008, 18, 5475.	6.7	64
33	QM/MM Study of the Role of the Solvent in the Formation of the Charge Separated Excited State in 9,9-Bianthryl. <i>Journal of the American Chemical Society</i> , 2005, 127, 11019-11028.	6.6	62
34	Solvent Effects on the $\pi^* \rightarrow n$ Transition of Acetone in Various Solvents: Direct Reaction Field Calculations. <i>Journal of Physical Chemistry A</i> , 1998, 102, 7984-7989.	1.1	61
35	The Formation and Recombination Kinetics of Positively Charged Poly(phenylene vinylene) Chains in Pulse-Irradiated Dilute Solutions. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5976-5986.	1.1	61
36	Mechanism of Charge Transport along Zinc Porphyrin-Based Molecular Wires. <i>Journal of the American Chemical Society</i> , 2009, 131, 5522-5529.	6.6	59

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37	Singlet Fission in Crystalline Organic Materials: Recent Insights and Future Directions. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 7208-7214.	2.1	59
38	Efficient Charge Transport along Phenylene-Vinylene Molecular Wires. <i>Journal of Physical Chemistry B</i> , 2006, 110, 14659-14666.	1.2	57
39	Enhanced charge-carrier mobility in $\pi^2$ -phase polyfluorene. <i>Physical Review B</i> , 2006, 74, .	1.1	55
40	Temperature Dependent Charge Carrier Dynamics in Formamidinium Lead Iodide Perovskite. <i>Journal of Physical Chemistry C</i> , 2017, 121, 23392-23397.	1.5	51
41	Computational Design of Two-Dimensional Perovskites with Functional Organic Cations. <i>Journal of Physical Chemistry C</i> , 2018, 122, 17118-17122.	1.5	51
42	Columnar Mesophases with 3D Order from New Functional Nonconventional Star-shaped Mesogens. <i>Advanced Materials</i> , 2008, 20, 4414-4418.	11.1	49
43	Hole Cooling Is Much Faster than Electron Cooling in PbSe Quantum Dots. <i>ACS Nano</i> , 2016, 10, 695-703.	7.3	49
44	Effect of intermolecular disorder on the intrachain charge transport in ladder-type poly(p-phenylenes). <i>Physical Review B</i> , 2006, 73, .	1.1	47
45	Efficient Charge Transport in Semisynthetic Zinc Chlorin Dye Assemblies. <i>Journal of the American Chemical Society</i> , 2012, 134, 16147-16150.	6.6	47
46	Frequency dependent mobility of charge carriers along polymer chains with finite length. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 382-386.	0.7	45
47	Electrochemical Control over Photoinduced Electron Transfer and Trapping in CdSe-CdTe Quantum-Dot Solids. <i>ACS Nano</i> , 2014, 8, 7067-7077.	7.3	42
48	Multi-layered hybrid perovskites templated with carbazole derivatives: optical properties, enhanced moisture stability and solar cell characteristics. <i>Journal of Materials Chemistry A</i> , 2018, 6, 22899-22908.	5.2	42
49	Electronic Structure and Optical Properties of Charged Oligofluorenes Studied by VIS/NIR Spectroscopy and Time-Dependent Density Functional Theory. <i>Journal of Physical Chemistry B</i> , 2006, 110, 5984-5993.	1.2	40
50	Self-assembly and semiconductivity of an oligothiophene supergelator. <i>Beilstein Journal of Organic Chemistry</i> , 2010, 6, 1070-1078.	1.3	40
51	Inducing Charge Separation in Solid-State Two-Dimensional Hybrid Perovskites through the Incorporation of Organic Charge-Transfer Complexes. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 824-830.	2.1	40
52	Charge Transport along Coiled Conjugated Polymer Chains. <i>Journal of Physical Chemistry C</i> , 2007, 111, 11104-11112.	1.5	39
53	Electronic Structure of Thienylene Vinylene Oligomers: Singlet Excited States, Triplet Excited States, Cations, and Dications. <i>Journal of Physical Chemistry B</i> , 2004, 108, 16139-16146.	1.2	38
54	Charge transfer versus molecular conductance: molecular orbital symmetry turns quantum interference rules upside down. <i>Chemical Science</i> , 2015, 6, 4196-4206.	3.7	38

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55	The effect of structural dimensionality on carrier mobility in lead-halide perovskites. <i>Journal of Materials Chemistry A</i> , 2019, 7, 23949-23957.	5.2	38
56	Positive Charge Carriers on Isolated Chains of MEHâˆ’PPV with Broken Conjugation:â€” Optical Absorption and Mobility. <i>Journal of Physical Chemistry B</i> , 2003, 107, 1554-1558.	1.2	36
57	Effect of GC Base Pairs on Charge Transfer through DNA Hairpins: The Importance of Electrostatic Interactions. <i>Journal of the American Chemical Society</i> , 2009, 131, 14204-14205.	6.6	36
58	Lead-Halide Perovskites Meet Donorâ€”Acceptor Charge-Transfer Complexes. <i>Chemistry of Materials</i> , 2019, 31, 6880-6888.	3.2	36
59	Electrodeless Measurement of the In-Plane Anisotropy in the Photoconductivity of an Aligned Polyfluorene Film. <i>Advanced Materials</i> , 2001, 13, 1627-1630.	11.1	35
60	Chemically Gated Quantum-Interference-Based Molecular Transistor. <i>Journal of Physical Chemistry Letters</i> , 2011, 2, 1753-1756.	2.1	35
61	Impact of the Computational Method on the Geometric and Electronic Properties of Oligo(phenylene) Tj ETQq1 1 0,784314 r <sub>g</sub> BT /Overl	1.2	34
62	The Relation between Rotational Dynamics of the Organic Cation and Phase Transitions in Hybrid Halide Perovskites. <i>Journal of Physical Chemistry C</i> , 2019, 123, 14652-14661.	1.5	34
63	Photogeneration and Mobility of Charge Carriers in Atomically Thin Colloidal InSe Nanosheets Probed by Ultrafast Terahertz Spectroscopy. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4191-4196.	2.1	33
64	Organic Field-Effect Transistors Utilizing Solution-Deposited Oligothiophene-Based Swivel Cruciforms. <i>Chemistry of Materials</i> , 2007, 19, 1267-1276.	3.2	30
65	High Electronic Conductance through Double-Helix DNA Molecules with Fullerene Anchoring Groups. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1182-1188.	1.1	30
66	Morphologyâ€”Independent Efficient Singlet Exciton Fission in Perylene Diimide Thin Films. <i>ChemPlusChem</i> , 2018, 83, 230-238.	1.3	30
67	Assessing the Role of Pt Clusters on TiO <sub>2</sub> (P25) on the Photocatalytic Degradation of Acid Blue 9 and Rhodamine B. <i>Journal of Physical Chemistry C</i> , 2020, 124, 8269-8278.	1.5	30
68	Interplay between Charge Carrier Mobility, Exciton Diffusion, Crystal Packing, and Charge Separation in Perylene Diimide-Based Heterojunctions. <i>ACS Applied Energy Materials</i> , 2019, 2, 8010-8021.	2.5	28
69	Cooling and Auger Recombination of Charges in PbSe Nanorods: Crossover from Cubic to Bimolecular Decay. <i>Nano Letters</i> , 2013, 13, 4380-4386.	4.5	26
70	Charge Transfer Through Molecules with Multiple Pathways: Quantum Interference and Dephasing. <i>Journal of Physical Chemistry C</i> , 2010, 114, 7973-7979.	1.5	25
71	Solid-State Infrared Upconversion in Perylene Diimides Followed by Direct Electron Injection. <i>ACS Energy Letters</i> , 2020, 5, 124-129.	8.8	25
72	Effect of Coâ€”Solvents on the Crystallization and Phase Distribution of Mixedâ€”Dimensional Perovskites. <i>Advanced Energy Materials</i> , 2021, 11, 2102144.	10.2	25

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73	Theoretical Study of the Optical Properties of Artificial Self-Assembled Zinc Chlorins. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20834-20842.	1.5	24
74	Perylene Bisimide Dyes with up to Five Independently Introduced Substituents: Controlling the Functionalization Pattern and Photophysical Properties Using Regiospecific Bay Substitution. <i>Journal of Organic Chemistry</i> , 2019, 84, 9532-9547.	1.7	24
75	Two-Dimensional Charge Delocalization in X-Shaped Phenylenevinylene Oligomers. <i>Chemistry of Materials</i> , 2006, 18, 2118-2129.	3.2	23
76	Opto-Electronic Properties of Fluorene-Based Derivatives as Precursors for Light-Emitting Diodes. <i>Journal of Physical Chemistry C</i> , 2007, 111, 5812-5820.	1.5	23
77	Effect of Electrostatic Interactions and Dynamic Disorder on the Distance Dependence of Charge Transfer in Donor-Bridge-Acceptor Systems. <i>Journal of Physical Chemistry B</i> , 2010, 114, 14564-14571.	1.2	22
78	Effect of Structural Dynamics and Base Pair Sequence on the Nature of Excited States in DNA Hairpins. <i>Journal of Physical Chemistry B</i> , 2012, 116, 11447-11458.	1.2	22
79	The effect of the magnitude and direction of the dipoles of organic cations on the electronic structure of hybrid halide perovskites. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 16564-16572.	1.3	22
80	Optical Properties and Delocalization of Excess Negative Charges on Oligo(Phenylenevinylene)s: A Quantum Chemical Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 5644-5652.	1.2	21
81	Single molecule charge transport: from a quantum mechanical to a classical description. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 2096-2110.	1.3	21
82	The relationship between molecular structure and electronic properties in dicyanovinyl substituted acceptor-donor-acceptor chromophores. <i>Tetrahedron</i> , 2017, 73, 4994-5004.	1.0	21
83	Relation between molecular packing and singlet fission in thin films of brominated perylenediimides. <i>Journal of Chemical Physics</i> , 2019, 151, 094301.	1.2	21
84	Potential and limitations of CsBi <sub>3</sub> I <sub>10</sub> as a photovoltaic material. <i>Journal of Materials Chemistry A</i> , 2020, 8, 15670-15674.	5.2	21
85	Trapping and Detrapping in Colloidal Perovskite Nanoplatelets: Elucidation and Prevention of Nonradiative Processes through Chemical Treatment. <i>Journal of Physical Chemistry C</i> , 2020, 124, 8047-8054.	1.5	21
86	Charge Photogeneration and Transport in AgBiS <sub>2</sub> Nanocrystal Films for Photovoltaics. <i>Solar Rrl</i> , 2019, 3, 1900075.	3.1	20
87	Tuning of the excited state properties of phenylenevinylene oligomers: A time-dependent density functional theory study. <i>Journal of Chemical Physics</i> , 2003, 118, 9441-9446.	1.2	19
88	Columnar Mesophases Based on Zinc Chlorophyll Derivatives Functionalized with Peripheral Dendron Wedges. <i>Chemistry - A European Journal</i> , 2011, 17, 5300-5310.	1.7	19
89	Limits of Defect Tolerance in Perovskite Nanocrystals: Effect of Local Electrostatic Potential on Trap States. <i>Journal of the American Chemical Society</i> , 2022, 144, 11059-11063.	6.6	19
90	Effects of the Environment on Charge Transport in Molecular Wires. <i>Journal of Physical Chemistry C</i> , 2012, 116, 25213-25225.	1.5	17

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91	Single-molecule functionality in electronic components based on orbital resonances. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 12849-12866.	1.3	17
92	2D layered perovskite containing functionalised benzothieno-benzothiophene molecules: formation, degradation, optical properties and photoconductivity. <i>Journal of Materials Chemistry C</i> , 2020, 8, 7181-7188.	2.7	17
93	Different Mechanisms for Hole and Electron Transfer along Identical Molecular Bridges: The Importance of the Initial State Delocalization. <i>Journal of Physical Chemistry A</i> , 2014, 118, 3891-3898.	1.1	16
94	Tailoring Photophysical Processes of Perylene-Based Light Harvesting Antenna Systems with Molecular Structure and Solvent Polarity. <i>Journal of Physical Chemistry C</i> , 2019, 123, 36-47.	1.5	16
95	Naphthalenediimide/Formamidineium-Based Low-Dimensional Perovskites. <i>Chemistry of Materials</i> , 2021, 33, 6412-6420.	3.2	16
96	Solvent Induced Charge Separation in the Excited States of Symmetrical Ethylene: A Direct Reaction Field Study. <i>Journal of Physical Chemistry A</i> , 2001, 105, 3583-3590.	1.1	15
97	Unravelling the structural complexity and photophysical properties of adamantyl-based layered hybrid perovskites. <i>Journal of Materials Chemistry A</i> , 2020, 8, 17732-17740.	5.2	14
98	Charge carrier dynamics in bulk poly(3-hexylthiophene) as a function of temperature. <i>Synthetic Metals</i> , 2001, 119, 431-432.	2.1	13
99	VIS/NIR Absorption Spectra of Positively Charged Oligo(phenylenevinylene)s and Comparison with Time-Dependent Density Functional Theory Calculations. <i>Journal of Physical Chemistry B</i> , 2004, 108, 19967-19975.	1.2	13
100	Charge transport along phenylenevinylene molecular wires. <i>Molecular Simulation</i> , 2006, 32, 695-705.	0.9	13
101	Optical and Conductive Properties of Large-Area Liquid Crystalline Monodomains of Terthiophene Derivatives. <i>Journal of Physical Chemistry C</i> , 2007, 111, 18411-18416.	1.5	13
102	Structural Dynamics of Two-Dimensional Ruddlesden-Popper Perovskites: A Computational Study. <i>Journal of Physical Chemistry C</i> , 2020, 124, 22096-22104.	1.5	13
103	Computational design of donor-bridge-acceptor systems exhibiting pronounced quantum interference effects. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 6773-6779.	1.3	12
104	Simulation of Hopping Transport Based on Charge Carrier Localization Times Derived for a Two-Level System. <i>Journal of Physical Chemistry C</i> , 2010, 114, 20424-20430.	1.5	11
105	High charge carrier mobility and efficient charge separation in highly soluble perylenetetra-carboxyl-diimides. <i>Chemical Communications</i> , 2014, 50, 4955-4958.	2.2	9
106	Structure-property relationships in multi-stimuli responsive BODIPY-biphenyl-benzodithiophene TICT rigidochromic rotors exhibiting (pseudo-)Stokes shifts up to 221 nm. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 25514-25521.	1.3	9
107	Tuning the Structural Rigidity of Two-Dimensional Ruddlesden-Popper Perovskites through the Organic Cation. <i>Journal of Physical Chemistry C</i> , 2020, 124, 28201-28209.	1.5	9
108	Frequency dependence of the charge carrier mobility in DH4T. <i>Synthetic Metals</i> , 2001, 119, 463-464.	2.1	6

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109	Dynamics and Lithium Binding Energies of Polyelectrolytes Based on Functionalized Poly(para-phenylene terephthalamide). <i>Journal of Physical Chemistry B</i> , 2005, 109, 7705-7712.	1.2	6
110	Engineering polymers with improved charge transport properties from bithiophene-containing polyamides. <i>Journal of Materials Chemistry C</i> , 2020, 8, 6281-6292.	2.7	5
111	Excited state dynamics of BODIPY-based acceptor–donor–acceptor systems: a combined experimental and computational study. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 8900-8907.	1.3	5
112	INS as a probe of inter-monomer angles in polymers. <i>Applied Physics A: Materials Science and Processing</i> , 2002, 74, s496-s498.	1.1	2
113	Radical Cations of All- <i>Trans</i> Oligodiacetylenes: Optical Absorption and Reactivity toward Nucleophiles. <i>Journal of Physical Chemistry B</i> , 2009, 113, 11095-11100.	1.2	2
114	Efficacious elimination of intramolecular charge transfer in perylene imide based light-harvesting antenna molecules. <i>Chemical Communications</i> , 2020, 56, 5560-5563.	2.2	2
115	Directing charge transfer in perylene based light-harvesting antenna molecules. <i>Journal of Chemical Physics</i> , 2020, 153, 144302.	1.2	1
116	Semiaromatic polyamides with enhanced charge carrier mobility. <i>Polymer Chemistry</i> , 2021, 12, 6914-6926.	1.9	1
117	A handle on charge reorganization. <i>Nature Chemistry</i> , 2022, 14, 720-722.	6.6	1
118	Mechanism and Absolute Rates of Charge Transfer Through DNA. <i>Nanoscience and Technology</i> , 2007, , 21-43.	1.5	0