

# Garth J Simpson

## List of Publications by Year in descending order

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133  
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#	ARTICLE	IF	CITATIONS
1	Supramolecular Assembly of His-Tagged Fluorescent Protein Guests within Coiled-Coil Peptide Crystal Hosts: Three-Dimensional Ordering and Protein Thermal Stability. <i>ACS Biomaterials Science and Engineering</i> , 2022, 8, 1860-1866.	2.6	2
2	Label-Free Autofluorescence-Detected Mid-Infrared Photothermal Microscopy of Pharmaceutical Materials. <i>Analytical Chemistry</i> , 2022, 94, 6512-6520.	3.2	8
3	Depth-of-field extension in optical imaging for rapid crystal screening. <i>Acta Crystallographica Section D: Structural Biology</i> , 2021, 77, 463-470.	1.1	0
4	Crystallization Kinetics in Fasted-State Simulated and Aspirated Human Intestinal Fluids. <i>Crystal Growth and Design</i> , 2021, 21, 2807-2820.	1.4	8
5	Fluorescence-Detected Mid-Infrared Photothermal Microscopy. <i>Journal of the American Chemical Society</i> , 2021, 143, 10809-10815.	6.6	27
6	Nonlinear optical characterization of pharmaceutical formulations. <i>TrAC - Trends in Analytical Chemistry</i> , 2021, 140, 116241.	5.8	7
7	Stochastic Differential Scanning Calorimetry by Nonlinear Optical Microscopy. <i>Analytical Chemistry</i> , 2020, 92, 1171-1178.	3.2	8
8	In Situ Crystal Growth Rate Distributions of Active Pharmaceutical Ingredients. <i>Molecular Pharmaceutics</i> , 2020, 17, 769-776.	2.3	6
9	Anomalous Diffusion Characterization by Fourier Transform-FRAP with Patterned Illumination. <i>Biophysical Journal</i> , 2020, 119, 737-748.	0.2	16
10	Disparities of Single-Particle Growth Rates in Buried Versus Exposed Ritonavir Crystals within Amorphous Solid Dispersions. <i>Molecular Pharmaceutics</i> , 2020, 17, 4564-4571.	2.3	5
11	Multiagent Consensus Equilibrium in Molecular Structure Determination. <i>Journal of Physical Chemistry A</i> , 2020, 124, 9105-9112.	1.1	0
12	Mueller Tensor Nonlinear Optical Polarization Analysis in Turbid Media. <i>Journal of Physical Chemistry B</i> , 2019, 123, 6643-6650.	1.2	5
13	Characterization of Phase Transformations for Amorphous Solid Dispersions of a Weakly Basic Drug upon Dissolution in Biorelevant Media. <i>Pharmaceutical Research</i> , 2019, 36, 174.	1.7	26
14	Iterative Non-Negative Matrix Factorization Filter for Blind Deconvolution in Photon/Ion Counting. <i>Analytical Chemistry</i> , 2019, 91, 5286-5294.	3.2	4
15	Axially-offset differential interference contrast microscopy via polarization wavefront shaping. <i>Optics Express</i> , 2019, 27, 3837.	1.7	8
16	Connecting Mueller and Jones tensors for describing nonlinear optical conversion of unpolarized light. , 2019, , .		0
17	Spatial encoded polarization dependent nonlinear optical analysis for local tensors imaging of collagenous tissue. , 2019, , .		0
18	Dynamic Sparse Sampling for Confocal Raman Microscopy. <i>Analytical Chemistry</i> , 2018, 90, 4461-4469.	3.2	25

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19	Triboluminescence from Pharmaceutical Formulations. <i>Analytical Chemistry</i> , 2018, 90, 6893-6898.	3.2	3
20	Kinetic Modeling of Accelerated Stability Testing Enabled by Second Harmonic Generation Microscopy. <i>Analytical Chemistry</i> , 2018, 90, 4406-4413.	3.2	10
21	Variation in Supersaturation and Phase Behavior of Ezetimibe Amorphous Solid Dispersions upon Dissolution in Different Biorelevant Media. <i>Molecular Pharmaceutics</i> , 2018, 15, 193-206.	2.3	21
22	Calibration-Free Second Harmonic Generation (SHG) Image Analysis for Quantification of Trace Crystallinity Within Final Dosage Forms of Amorphous Solid Dispersions. <i>Applied Spectroscopy</i> , 2018, 72, 1594-1605.	1.2	7
23	Spatially encoded polarization-dependent nonlinear optics. <i>Optics Letters</i> , 2018, 43, 5973.	1.7	2
24	Mueller tensor approach for nonlinear optics in turbid media. , 2018, , .		0
25	Dynamic sparse sampling in Raman imaging. , 2018, , .		0
26	Spatiotemporal polarization modulation microscopy with a microretarder array. , 2018, , .		0
27	Dynamic X-ray diffraction sampling for protein crystal positioning. <i>Journal of Synchrotron Radiation</i> , 2017, 24, 188-195.	1.0	19
28	Second Harmonic Generation Guided Raman Spectroscopy for Sensitive Detection of Polymorph Transitions. <i>Analytical Chemistry</i> , 2017, 89, 5958-5965.	3.2	12
29	Second harmonic generation microscopy as a tool for the early detection of crystallization in spray dried dispersions. <i>Journal of Pharmaceutical and Biomedical Analysis</i> , 2017, 146, 86-95.	1.4	22
30	Second Harmonic Generation of Unpolarized Light. <i>Physical Review Letters</i> , 2017, 119, 193901.	2.9	15
31	Spatial-spectral multiplexing for hyperspectral multiphoton fluorescence imaging. <i>Optics Express</i> , 2017, 25, 32243.	1.7	8
32	Synchrotron X-Ray Diffraction Dynamic Sampling for Protein Crystal Centering. <i>IS&amp;T International Symposium on Electronic Imaging</i> , 2017, 29, 6-9.	0.3	2
33	Guiding synchrotron X-ray diffraction by multimodal video-rate protein crystal imaging. <i>Journal of Synchrotron Radiation</i> , 2016, 23, 959-965.	1.0	8
34	Connection of Jones and Mueller Tensors in Second Harmonic Generation and Multi-Photon Fluorescence Measurements. <i>Journal of Physical Chemistry B</i> , 2016, 120, 3281-3302.	1.2	17
35	Rapid Discrimination of Polymorphic Crystal Forms by Nonlinear Optical Stokes Ellipsometric Microscopy. <i>Analytical Chemistry</i> , 2016, 88, 5760-5768.	3.2	19
36	Theoretical Foundation for Electric-Dipole-Allowed Chiral-Specific Fluorescence Optical Rotary Dispersion (F-ORD) from Interfacial Assemblies. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4248-4252.	2.1	2

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37	Imaging the Nonlinear Susceptibility Tensor of Collagen by Nonlinear Optical Stokes Ellipsometry. <i>Biophysical Journal</i> , 2016, 111, 1361-1374.	0.2	26
38	Unified Theory for Polarization Analysis in Second Harmonic and Sum Frequency Microscopy. <i>Biophysical Journal</i> , 2016, 111, 1553-1568.	0.2	18
39	Nonlinear Optical Characterization of Membrane Protein Microcrystals and Nanocrystals. <i>Advances in Experimental Medicine and Biology</i> , 2016, 922, 91-103.	0.8	3
40	Second harmonic generation correlation spectroscopy for characterizing translationally diffusing protein nanocrystals. <i>Acta Crystallographica Section D: Structural Biology</i> , 2016, 72, 849-859.	1.1	1
41	Powders Analysis by Second Harmonic Generation Microscopy. <i>Analytical Chemistry</i> , 2016, 88, 3853-3863.	3.2	19
42	Drop printing of pharmaceuticals: Effect of molecular weight on PEG coated naproxen/PEG 3350 solid dispersions. <i>AIChE Journal</i> , 2015, 61, 4502-4508.	1.8	22
43	Spectral x-ray diffraction using a 6 megapixel photon counting array detector. , 2015, 9401, 940109.		0
44	Synchronous-digitization for video rate polarization modulated beam scanning second harmonic generation microscopy. <i>Proceedings of SPIE</i> , 2015, 9330, 93300A.	0.8	1
45	Imaging local electric fields produced upon synchrotron X-ray exposure. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 696-701.	3.3	9
46	Ab Initio Prediction of the Diversity of Second Harmonic Generation from Pharmaceutically Relevant Materials. <i>Crystal Growth and Design</i> , 2015, 15, 581-586.	1.4	16
47	Multi-channel beam-scanning imaging at kHz frame rates by Lissajous trajectory microscopy. , 2015, 9330, 933009.		2
48	Finding the Needle in the Haystack: Characterization of Trace Crystallinity in a Commercial Formulation of Paclitaxel Protein-Bound Particles by Raman Spectroscopy Enabled by Second Harmonic Generation Microscopy. <i>Molecular Pharmaceutics</i> , 2015, 12, 2378-2383.	2.3	34
49	Video-rate two-photon excited fluorescence lifetime imaging system with interleaved digitization. <i>Optics Letters</i> , 2015, 40, 3296.	1.7	17
50	Parts per Million Powder X-ray Diffraction. <i>Analytical Chemistry</i> , 2015, 87, 10950-10955.	3.2	70
51	Intercalating dyes for enhanced contrast in second-harmonic generation imaging of protein crystals. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2015, 71, 1471-1477.	2.5	4
52	High frame-rate multichannel beam-scanning microscopy based on Lissajous trajectories. <i>Optics Express</i> , 2014, 22, 24224.	1.7	57
53	Synchronous digitization for high dynamic range lock-in amplification in beam-scanning microscopy. <i>Review of Scientific Instruments</i> , 2014, 85, 033703.	0.6	20
54	Water-solid interactions in amorphous maltodextrin-crystalline sucrose binary mixtures. <i>Pharmaceutical Development and Technology</i> , 2014, 19, 247-256.	1.1	17

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55	Kinetic Trapping of Metastable Amino Acid Polymorphs. <i>Journal of the American Chemical Society</i> , 2014, 136, 2404-2412.	6.6	28
56	Digital Deconvolution Filter Derived from Linear Discriminant Analysis and Application for Multiphoton Fluorescence Microscopy. <i>Analytical Chemistry</i> , 2014, 86, 3508-3516.	3.2	5
57	Exciton Coupling Model for the Emergence of Second Harmonic Generation from Assemblies of Centrosymmetric Molecules. <i>Journal of Physical Chemistry A</i> , 2014, 118, 4301-4308.	1.1	0
58	Polarization-Modulated Second Harmonic Generation Ellipsometric Microscopy at Video Rate. <i>Analytical Chemistry</i> , 2014, 86, 8448-8456.	3.2	41
59	Impact of Polymers on the Precipitation Behavior of Highly Supersaturated Aqueous Danazol Solutions. <i>Molecular Pharmaceutics</i> , 2014, 11, 3027-3038.	2.3	57
60	Linear fitting of multi-threshold counting data with a pixel-array detector for spectral X-ray imaging. <i>Journal of Synchrotron Radiation</i> , 2014, 21, 1180-1187.	1.0	2
61	Crystallization and Dissolution Behavior of Naproxen/Polyethylene Glycol Solid Dispersions. <i>Journal of Physical Chemistry B</i> , 2013, 117, 1494-1500.	1.2	38
62	Effect of Substrates on Naproxen-Polyvinylpyrrolidone Solid Dispersions Formed via the Drop Printing Technique. <i>Journal of Pharmaceutical Sciences</i> , 2013, 102, 638-648.	1.6	41
63	Integrated nonlinear optical imaging microscope for on-axis crystal detection and centering at a synchrotron beamline. <i>Journal of Synchrotron Radiation</i> , 2013, 20, 531-540.	1.0	31
64	Polarization-resolved second-harmonic generation microscopy as a method to visualize protein-crystal domains. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 74-81.	2.5	29
65	Development of a High-Throughput Laser-Induced Acoustic Desorption Probe and Raster Sampling For Laser-Induced Acoustic Desorption/Atmospheric Pressure Chemical Ionization. <i>Analytical Chemistry</i> , 2013, 85, 5720-5726.	3.2	16
66	Real-time dynamic range and signal to noise enhancement in beam-scanning microscopy by integration of sensor characteristics, data acquisition hardware, and statistical methods. <i>Proceedings of SPIE</i> , 2013, 8657, 86570E.	0.8	6
67	Stimulated Raman scattering imaging by continuous-wave laser excitation. <i>Optics Letters</i> , 2013, 38, 1479.	1.7	36
68	Towards protein-crystal centering using second-harmonic generation (SHG) microscopy. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2013, 69, 843-851.	2.5	30
69	Statistical connection of binomial photon counting and photon averaging in high dynamic range beam-scanning microscopy. <i>Optics Express</i> , 2012, 20, 10406.	1.7	19
70	Modeling the SHG activities of diverse protein crystals. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2012, 68, 1513-1521.	2.5	22
71	Nonlinear Optical Imaging for Sensitive Detection of Crystals in Bulk Amorphous Powders. <i>Journal of Pharmaceutical Sciences</i> , 2012, 101, 4201-4213.	1.6	43
72	Second-Order Nonlinear Optical Imaging of Chiral Crystals. <i>Annual Review of Analytical Chemistry</i> , 2011, 4, 419-437.	2.8	115

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73	Mining the polarization-dependence of nonlinear optical measurements. <i>Analyst, The</i> , 2011, 136, 652-662.	1.7	12
74	Screening of protein crystallization trials by second order nonlinear optical imaging of chiral crystals (SONICC). <i>Methods</i> , 2011, 55, 379-386.	1.9	50
75	Computational Investigation of Amine-Oxygen Exciplex Formation. <i>Journal of Physical Chemistry A</i> , 2011, 115, 10159-10165.	1.1	11
76	Two-photon excited UV fluorescence for protein crystal detection. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2011, 67, 839-846.	2.5	45
77	Chemically Selective Analysis of Molecular Monolayers by Nonlinear Optical Stokes Ellipsometry. <i>Analytical Chemistry</i> , 2010, 82, 559-566.	3.2	9
78	Statistical Treatment of Photon/Electron Counting: Extending the Linear Dynamic Range from the Dark Count Rate to Saturation. <i>Analytical Chemistry</i> , 2010, 82, 10129-10134.	3.2	27
79	Direct Observation of Transient Ostwald Crystallization Ordering from Racemic Serine Solutions. <i>Journal of the American Chemical Society</i> , 2010, 132, 13598-13599.	6.6	23
80	Selective Detection and Quantitation of Organic Molecule Crystallization by Second Harmonic Generation Microscopy. <i>Analytical Chemistry</i> , 2010, 82, 5425-5432.	3.2	68
81	Nonlinear Optical Imaging of Integral Membrane Protein Crystals in Lipidic Mesophases. <i>Analytical Chemistry</i> , 2010, 82, 491-497.	3.2	68
82	DNA-Based Polymers as Chiral Templates for Second-Order Nonlinear Optical Materials. <i>ChemPhysChem</i> , 2009, 10, 2674-2678.	1.0	20
83	Nonlinear Optical Stokes Ellipsometry. 1. Theoretical Framework. <i>Journal of Physical Chemistry C</i> , 2009, 113, 10158-10165.	1.5	22
84	Nonlinear Optical Stokes Ellipsometry. 2. Experimental Demonstration. <i>Journal of Physical Chemistry C</i> , 2009, 113, 10166-10175.	1.5	23
85	Chirality in Nonlinear Optics. <i>Annual Review of Physical Chemistry</i> , 2009, 60, 345-365.	4.8	131
86	An electrochemical fabrication process for the assembly of anisotropically oriented collagen bundles. <i>Biomaterials</i> , 2008, 29, 3278-3288.	5.7	224
87	Polarization-dependent two-photon absorption for the determination of protein secondary structure: A theoretical study. <i>Chemical Physics Letters</i> , 2008, 455, 6-12.	1.2	29
88	Interpreting nonlinear optics of biopolymer assemblies: Finding a hook. <i>Chemical Physics Letters</i> , 2008, 465, 167-174.	1.2	24
89	Molecular Design Strategies for Optimizing the Nonlinear Optical Properties of Chiral Crystals. <i>Crystal Growth and Design</i> , 2008, 8, 2589-2594.	1.4	35
90	Assembly of Dithiocarbamate-Anchored Monolayers on Gold Surfaces in Aqueous Solutions. <i>Langmuir</i> , 2008, 24, 8660-8666.	1.6	57

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91	Molecular Self-Assembly of Mixed High-Beta Zwitterionic and Neutral Ground-State NLO Chromophores. <i>Chemistry of Materials</i> , 2008, 20, 1778-1787.	3.2	31
92	Selective Detection of Protein Crystals by Second Harmonic Microscopy. <i>Journal of the American Chemical Society</i> , 2008, 130, 14076-14077.	6.6	109
93	Selection Rules and Symmetry Relations for Four-Wave Mixing Measurements of Uniaxial Assemblies. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5834-5848.	1.2	31
94	Discrete retardance second harmonic generation ellipsometry. <i>Review of Scientific Instruments</i> , 2007, 78, 013106.	0.6	9
95	Visual Methods for Interpreting Optical Nonlinearity at the Molecular Level. <i>Accounts of Chemical Research</i> , 2007, 40, 953-960.	7.6	45
96	NLOPredict: Visualization and data analysis software for nonlinear optics. <i>Journal of Computational Chemistry</i> , 2007, 28, 1996-2002.	1.5	30
97	Nanoscale Dielectrophoretic Spectroscopy of Individual Immobilized Mammalian Blood Cells. <i>Biophysical Journal</i> , 2006, 91, 2678-2686.	0.2	16
98	Mechanism of the Chiral SHG Activity of Bacteriorhodopsin Films. <i>Journal of the American Chemical Society</i> , 2006, 128, 10994-10995.	6.6	32
99	The diffraction barrier broken. <i>Nature</i> , 2006, 440, 879-880.	13.7	8
100	Modular ellipsometric approach for mining structural information from nonlinear optical polarization analysis. <i>Physical Review B</i> , 2005, 72, .	1.1	28
101	Self-Consistent Approach for Simplifying the Molecular Interpretation of Nonlinear Optical and Multiphoton Phenomena. <i>Journal of Physical Chemistry A</i> , 2005, 109, 1316-1323.	1.1	36
102	Electronic and Vibrational Second-Order Nonlinear Optical Properties of Protein Secondary Structural Motifs. <i>Journal of Physical Chemistry B</i> , 2005, 109, 20009-20026.	1.2	76
103	Direct Determination of Effective Interfacial Optical Constants by Nonlinear Optical Null Ellipsometry of Chiral Films. <i>Analytical Chemistry</i> , 2005, 77, 215-224.	3.2	33
104	Reduction of Tip-Sample Contact Using Dielectrophoretic Force Scanning Probe Microscopy. <i>Analytical Chemistry</i> , 2005, 77, 8008-8012.	3.2	11
105	Dielectrophoretic Force Microscopy of Aqueous Interfaces. <i>Langmuir</i> , 2005, 21, 1436-1440.	1.6	11
106	Molecular Origins of the Remarkable Chiral Sensitivity of Second-Order Nonlinear Optics. <i>ChemPhysChem</i> , 2004, 5, 1301-1310.	1.0	122
107	The general failure of Kleinman symmetry in practical nonlinear optical applications. <i>Chemical Physics Letters</i> , 2004, 390, 8-13.	1.2	67
108	Uncoupled oscillator model for interpreting second harmonic generation measurements of oriented chiral systems. <i>Chemical Physics Letters</i> , 2004, 399, 26-32.	1.2	20

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109	Ellipsometric Approach for the Real-Time Detection of Label-Free Protein Adsorption by Second Harmonic Generation. <i>Journal of the American Chemical Society</i> , 2004, 126, 5001-5007.	6.6	44
110	A Unified Treatment of Selection Rules and Symmetry Relations for Sum-Frequency and Second Harmonic Spectroscopies. <i>Journal of Physical Chemistry B</i> , 2004, 108, 3548-3562.	1.2	263
111	The molecular origins of optical nonlinearity: beyond charge-transfer effects. , 2004, 5517, 106.		0
112	Polarization characterization in surface second harmonic generation by nonlinear optical null ellipsometry. <i>Analytica Chimica Acta</i> , 2003, 496, 133-142.	2.6	29
113	Experimental Confirmation of the Importance of Orientation in the Anomalous Chiral Sensitivity of Second Harmonic Generation. <i>Journal of the American Chemical Society</i> , 2003, 125, 9111-9115.	6.6	56
114	Molecular and surface hyperpolarizability of oriented chromophores of low symmetry. <i>Physical Review B</i> , 2002, 66, .	1.1	40
115	Irradiation of Dye-Doped Microspheres with a Strongly Focused Laser Beam Results in Alignment upon Optical Trapping. <i>Nano Letters</i> , 2002, 2, 207-210.	4.5	3
116	Coupled Electrorotation of Polymer Microspheres for Microfluidic Sensing and Mixing. <i>Analytical Chemistry</i> , 2002, 74, 5099-5104.	3.2	17
117	Structural origins of circular dichroism in surface second harmonic generation. <i>Journal of Chemical Physics</i> , 2002, 117, 3398-3410.	1.2	56
118	Coupled Electrorotation: Two Proximate Microspheres Spin in Registry with an AC Electric Field. <i>ChemPhysChem</i> , 2002, 3, 416.	1.0	15
119	New Tools for Surface Second-Harmonic Generation. <i>Applied Spectroscopy</i> , 2001, 55, 16A-32A.	1.2	24
120	Nanoengineered Structures for Holding and Manipulating Liposomes and Cells. <i>Analytical Chemistry</i> , 2001, 73, 787-791.	3.2	19
121	Influence of substrate roughness on orientation measurements by second-harmonic generation. <i>Chemical Physics Letters</i> , 2000, 317, 276-281.	1.2	10
122	Orientation-Insensitive Methodology for Second Harmonic Generation. 1. Theory. <i>Analytical Chemistry</i> , 2000, 72, 3399-3406.	3.2	24
123	Molecular Orientation and Angular Distribution Probed by Angle-Resolved Absorbance and Second Harmonic Generation. <i>Analytical Chemistry</i> , 2000, 72, 887-898.	3.2	68
124	Orientation-Insensitive Methodology for Second Harmonic Generation. 2. Application to Adsorption Isotherm and Kinetics Measurements. <i>Analytical Chemistry</i> , 2000, 72, 3407-3411.	3.2	31
125	Measurement of Orientation in Organic Thin Films. <i>Accounts of Chemical Research</i> , 2000, 33, 781-789.	7.6	50
126	Evaluation of molecular-scale roughness at liquid interfaces. <i>Chemical Physics Letters</i> , 1999, 309, 117-122.	1.2	24



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127	Surface Roughness by Contact versus Tapping Mode Atomic Force Microscopy. <i>Langmuir</i> , 1999, 15, 1429-1434.	1.6	73
128	Molecular Orientation at Surfaces: Surface Roughness Contributions to Measurements Based on Linear Dichroism. <i>Journal of Physical Chemistry B</i> , 1999, 103, 3800-3811.	1.2	25
129	Quantification of "Local" Surface Orientation: Theory and Experiment. <i>Journal of Physical Chemistry B</i> , 1999, 103, 1525-1531.	1.2	26
130	An SHG Magic Angle: Dependence of Second Harmonic Generation Orientation Measurements on the Width of the Orientation Distribution. <i>Journal of the American Chemical Society</i> , 1999, 121, 2635-2636.	6.6	157
131	Evolution of Orientation in the Growth of Azo Dye Zirconium Phosphate/Phosphonate Multilayers. <i>Journal of the American Chemical Society</i> , 1998, 120, 7997-7998.	6.6	17
132	Infrared Spectroscopy and Temperature-Programmed Desorption Study of Adsorbed Thiophene on $\gamma$ -Al <sub>2</sub> O <sub>3</sub> . <i>Langmuir</i> , 1996, 12, 1500-1510.	1.6	35
133	Thiophene Hydrodesulfurization over Alumina-Supported Molybdenum Carbide and Nitride Catalysts: Adsorption Sites, Catalytic Activities, and Nature of the Active Surface. <i>Journal of Catalysis</i> , 1996, 164, 109-121.	3.1	184