Julio R Sambrano

List of Publications by Year
in descending order

140 papers	3,813 citations	136950 32 h-index	161849 54 g-index
141 all docs	141 docs citations	141 times ranked	4089 citing authors

#	Article	IF	Citations
1	Structural and optical properties of CaTiO3 perovskite-based materials obtained by microwave-assisted hydrothermal synthesis: An experimental and theoretical insight. Acta Materialia, 2009, 57, 5174-5185.	7.9	194
2	Electronic structure and optical properties of BaMoO4 powders. Current Applied Physics, 2010, 10, 614-624.	2.4	150
3	Strong violetâ€“blue light photoluminescence emission at room temperature in SrZrO3: Joint experimental and theoretical study. Acta Materialia, 2008, 56, 2191-2202.	7.9	132
4	Static simulation of bulk and selected surfaces of anatase TiO2. Surface Science, 2001, 490, 116-124.	1.9	115
5	Different Origins of Green-Light Photoluminescence Emission in Structurally Ordered and Disordered Powders of Calcium Molybdate. Journal of Physical Chemistry A, 2008, 112, 8920-8928.	2.5	112
6	Highly intense violet-blue light emission at room temperature in structurally disordered SrZrO3 powders. Applied Physics Letters, 2007, 90, 091906.	3.3	109
7	Synthesis of wurtzite ZnS nanoparticles using the microwave assisted solvothermal method. Journal of Alloys and Compounds, 2013, 556, 153-159.	5.5	105
8	Periodic study on the structural and electronic properties of bulk, oxidized and reduced SnO 2 (1 1 0) surfaces and the interaction with O 2. Surface Science, 2002, 511, 408-420.	1.9	100
9	Zinc blende versus wurtzite ZnS nanoparticles: control of the phase and optical properties by tetrabutylammonium hydroxide. Physical Chemistry Chemical Physics, 2014, 16, 20127-20137.	2.8	100
10	CeO₂ Nanoparticle Morphologies and Their Corresponding Crystalline Planes for the Photocatalytic Degradation of Organic Pollutants. ACS Applied Nano Materials, 2019, 2, 6513-6526.	5.0	87
11	Experimental and theoretical correlation of very intense visible green photoluminescence in BaZrO3 powders. Journal of Applied Physics, 2008, 103, .	2.5	84
12	Electronic and Structural Properties of the (101Ì…0) and (112Ì…0) ZnO Surfaces. Journal of Physical Chemistry A, 2008, 112, 8958-8963.	2.5	83
13	Theoretical Study on the Molecular Mechanism for the Reaction of VO2+ with C2H4. Journal of Physical Chemistry A, 2003, 107, 3107-3120.	2.5	68
14	Density Functional Theory Study on the Structural and Electronic Properties of Low Index Rutile Surfaces for TiO₂/SnO₂/TiO₂ and SnO₂/TiO₂/SnO₂ Composite Systems. Journal of Physical Chemistry A, 2008, 112, 8943-8952.	2.5	65
15	Toward an Understanding of Intermediate- and Short-Range Defects in ZnO Single Crystals. A Combined Experimental and Theoretical Study. Journal of Physical Chemistry A, 2008, 112, 8970-8978.	2.5	64
16	Structural and electronic properties of PbTiO3 slabs: a DFT periodic study. Surface Science, 2004, 552, 149-159.	1.9	62
17	A theoretical study on cytosine tautomers in aqueous media by using continuum models. Chemical Physics Letters, 2000, 317, 437-443.	2.6	61
18	DFT Study of the Reaction between VO2+ and C2H6. Organometallics, 2004, 23, 730-739.	2.3	61

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19	Intense violetâ€“blue photoluminescence in BaZrO3 powders: A theoretical and experimental investigation of structural orderâ€“disorder. Optics Communications, 2008, 281, 3715-3720.	2.1	52
20	A theoretical and experimental investigation of Eu-doped ZnO nanorods and its application on dye sensitized solar cells. Journal of Alloys and Compounds, 2018, 739, 939-947.	5.5	52
21	DFT Study on Ce-Doped Anatase TiO₂: Nature of Ce³⁺ and Ti³⁺ Centers Triggered by Oxygen Vacancy Formation. Journal of Physical Chemistry C, 2014, 118, 9677-9689.	3.1	51
22	Electronic and structural properties of the (001) SrZrO3 surface. Computational and Theoretical Chemistry, 2007, 813, 49-56.	1.5	50
23	Role of Surfaces in the Magnetic and Ozone Gas-Sensing Properties of ZnFe₂O₄ Nanoparticles: Theoretical and Experimental Insights. ACS Applied Materials & Interfaces, 2021, 13, 4605-4617.	8.0	49
24	Theoretical analysis of the structural deformation in Mn-doped BaTiO3. Chemical Physics Letters, 2005, 402, 491-496.	2.6	47
25	A <scp>DFT</scp> Study of Structural and Electronic Properties of <scp><scp>ZnS</scp></scp> Polymorphs and its Pressureâ€Induced Phase Transitions. Journal of the American Ceramic Society, 2014, 97, 4011-4018.	3.8	43
26	A theoretical analysis of the TiO2/Sn doped (110) surface properties. Surface Science, 2005, 580, 71-79.	1.9	42
27	Strutural and optical approach of CdS@ZnS coreâ€“shell system. Chemical Physics Letters, 2012, 536, 96-99.	2.6	37
28	Theoretical study of the structure and stability of NbxOy and NbxOy+ (x=1â€“3; y=2â€“5,â€˜7,â€˜8) clusters. Chemical Physics Letters, 1998, 287, 620-626.	2.6	36
29	Î±-Ag_{2â€“2x}Zn_xWO₄ (0 â‰¤ x â‰¤ 0.25) Solid Solutions: Structure, Morphology, and Optical Properties. Inorganic Chemistry, 2017, 56, 7360-7372.	4.0	36
30	TiO2 synthesized by microwave assisted solvothermal method: Experimental and theoretical evaluation. Journal of Solid State Chemistry, 2014, 210, 171-177.	2.9	34
31	Modeling the atomic-scale structure, stability, and morphological transformations in the tetragonal phase of LaVO4. Chemical Physics Letters, 2016, 660, 87-92.	2.6	34
32	Adsorption of NH₃ with Different Coverages on Single-Walled ZnO Nanotube: DFT and QTAIM Study. Journal of Physical Chemistry C, 2017, 121, 8109-8119.	3.1	34
33	Density functional study of the 5-methylcytosine tautomers. Chemical Physics, 2001, 264, 333-340.	1.9	33
34	Structural, electronic and mechanical properties of single-walled AlN and GaN nanotubes via DFT/B3LYP. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	33
35	Hydrothermal synthesis, structural characterization and photocatalytic properties of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mi>Î²</mml:mi></mml:math>-Ag2MoO4 microcrystals: Correlation between experimental and theoretical data. Arabian Journal of Chemistry, 2020, 13, 2806-2825.	4.9	33
36	Correlation between structural and electronic orderâ€“disorder effects and optical properties in ZnO nanocrystals. Journal of Materials Chemistry C, 2014, 2, 10164-10174.	5.5	31

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37	Theoretical methods for calculations of optical phonons in BiOBr: Analysis and correction of propagated errors. Journal of Raman Spectroscopy, 2018, 49, 1356-1363.	2.5	31
38	DFT Study with Inclusion of the Grimme Potential on Anatase TiO₂: Structure, Electronic, and Vibrational Analyses. Journal of Physical Chemistry A, 2012, 116, 11731-11735.	2.5	30
39	Optical and gas-sensing properties, and electronic structure of the mixed-phase CaCu 3 Ti 4 O 12 /CaTiO 3 composites. Materials Research Bulletin, 2017, 93, 47-55.	5.2	30
40	Mechanistic Insights into the Reaction between VO2+ and Propene Based on a DFT Study. Organometallics, 2006, 25, 1643-1653.	2.3	28
41	In silico infrared and Raman spectroscopy under pressure: The case of CaSnO3 perovskite. Journal of Chemical Physics, 2015, 142, 014505.	3.0	28
42	Antimicrobial activity of TiO2:Ag nanocrystalline heterostructures: Experimental and theoretical insights. Chemical Physics, 2015, 459, 87-95.	1.9	28
43	Structural, Electronic, Vibrational, and Topological Analysis of Single-Walled Zinc Oxide Nanotubes. Journal of Physical Chemistry C, 2016, 120, 6814-6823.	3.1	28
44	Joint Experimental and Theoretical Analysis of Orderâ^'Disorder Effects in Cubic BaZrO₃ Assembled Nanoparticles under Decaoctahedral Shape. Journal of Physical Chemistry A, 2011, 115, 4482-4490.	2.5	27
45	Theoretical study of porous surfaces derived from graphene and boron nitride. Journal of Solid State Chemistry, 2018, 258, 247-255.	2.9	27
46	A Theoretical Study on the Gas Phase Reactions of the Anions NbO3-, NbO5-, and NbO2(OH)2- with H2O and O2. Journal of Physical Chemistry A, 2004, 108, 10850-10860.	2.5	26
47	Experimental and theoretical studies on the enhanced photoluminescence activity of zinc sulfide with a capping agent. Journal of Applied Physics, 2011, 110, 123507.	2.5	26
48	DFT study of the water-assisted tautomerization process between hydrated oxide, MO(H2O)+, and dihydroxide, M(OH)2+, cations (M=V, Nb and Ta). Chemical Physics Letters, 2004, 384, 56-62.	2.6	25
49	Photocatalytic activity of semiconductor sulfide heterostructures. Dalton Transactions, 2013, 42, 11111.	3.3	25
50	Oxidative dehydrogenation of ethylbenzene to styrene over the CoFe2O4â€“MCM-41 catalyst: preferential adsorption on the O2â^'Fe3+O2â^' sites located at octahedral positions. Catalysis Science and Technology, 2019, 9, 2469-2484.	4.1	25
51	Cation-exchange mediated synthesis of hydrogen and sodium titanates heterojunction: Theoretical and experimental insights toward photocatalyic mechanism. Applied Surface Science, 2021, 538, 148137.	6.1	25
52	Influence of solvent on the morphology and photocatalytic properties of ZnS decorated CeO2 nanoparticles. Journal of Applied Physics, 2014, 115, .	2.5	24
53	Theoretical Study of the Stoichiometric and Reduced Ce-Doped TiO2Anatase (001) Surfaces. Journal of Physical Chemistry C, 2015, 119, 4805-4816.	3.1	24
54	Decay of photo-induced conductivity in Sb-doped SnO2 thin films, using monochromatic light of about bandgap energy. Applied Surface Science, 2013, 267, 164-168.	6.1	23

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55	Preparation of TiO₂/SnO₂ Thin Films by Solâ€“Gel Method and Periodic B3LYP Simulations. Journal of Physical Chemistry A, 2014, 118, 5857-5865.	2.5	23
56	Periodic density functional theory study of structural and electronic properties of single-walled zinc oxide and carbon nanotubes. Journal of Solid State Chemistry, 2016, 237, 36-47.	2.9	23
57	Thermal properties of the orthorhombic CaSnO3 perovskite under pressure from ab initio quasi-harmonic calculations. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	22
58	Quantitative evaluation of the surface stability and morphological changes of Cu2O particles. Heliyon, 2019, 5, e02500.	3.2	22
59	Influence of Synthesis Time on the Morphology and Properties of CeO₂ Nanoparticles: An Experimentalâ€“Theoretical Study. Crystal Growth and Design, 2020, 20, 5031-5042.	3.0	22
60	Theoretical analysis of the energy levels induced by oxygen vacancies and the doping process (Co, Cu) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.3	21
61	Probing the Site-Selective Doping in SrSnO₃:Eu Oxides and Its Impact on the Crystal and Electronic Structures Using Synchrotron Radiation and DFT Simulations. Inorganic Chemistry, 2020, 59, 7666-7680.	4.0	21
62	Band Gap Narrowing of Bi-Doped NaTaO₃ for Photocatalytic Hydrogen Evolution under Simulated Sunlight: A Pseudocubic Phase Induced by Doping. ACS Applied Energy Materials, 2021, 4, 671-679.	5.1	21
63	Hydrostatic and [001] Uniaxial Pressure on Anatase TiO₂ by Periodic B3LYP-D* Calculations. Journal of Physical Chemistry C, 2013, 117, 7050-7061.	3.1	20
64	Computational Simulations of Morphological Transformations by Surface Structures: The Case of Rutile TiO2 phase. Materials Research, 2017, 20, 920-925.	1.3	20
65	Spin-phonon coupling in uniaxial anisotropic spin-glass based on Fe2TiO5 pseudobrookite. Journal of Alloys and Compounds, 2019, 799, 563-572.	5.5	20
66	Evaluation of bulk and surfaces absorption edge energy of sol-gel-dip-coating SnO2 thin films. Materials Research, 2010, 13, 437-443.	1.3	19
67	A DFT rationalization of the room temperature photoluminescence of Li2TiSiO5. Chemical Physics Letters, 2004, 398, 330-335.	2.6	18
68	Structural, electronic and optical properties of Fe(III) complex with pyridine-2,6-dicarboxylic acid: A combined experimental and theoretical study. Inorganica Chimica Acta, 2014, 416, 200-206.	2.4	17
69	Europium doped zinc sulfide: a correlation between experimental and theoretical calculations. Journal of Molecular Modeling, 2014, 20, 2375.	1.8	17
70	Porous silicene and silicon graphenylene-like surfaces: a DFT study. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	17
71	Computational procedure to an accurate DFT simulation to solid state systems. Computational Materials Science, 2019, 170, 109176.	3.0	17
72	An ab initio study of oxygen vacancies and doping process of Nb and Cr atoms on TiO2 (110) surface models. International Journal of Quantum Chemistry, 1997, 65, 625-631.	2.0	16

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73	A theoretical analysis on electronic structure of the (110) surface of TiO2â€“SnO2 mixed oxide. Computational and Theoretical Chemistry, 2003, 629, 307-314.	1.5	16
74	Pb1â^'xCaxTiO3solid solution (x=0.0, 0.25, 0.50, and 0.75): A theoretical and experimental approach. Physical Review B, 2007, 75, .	3.2	16
75	Theoretical Study on the Reaction Mechanism of VO₂⁺ with Propyne in Gas Phase. Journal of Physical Chemistry A, 2008, 112, 1808-1816.	2.5	16
76	Piezoelectric, elastic, Infrared and Raman behavior of ZnO wurtzite under pressure from periodic DFT calculations. Chemical Physics, 2017, 485-486, 98-107.	1.9	16
77	A theoretical analysis on the intramolecular proton transfer of Î±-alanine in an aqueous medium. Chemical Physics Letters, 1998, 294, 1-8.	2.6	15
78	Experimental and theoretical approach of nanocrystalline TiO2 with antifungal activity. Chemical Physics Letters, 2013, 577, 114-120.	2.6	14
79	New two-dimensional zinc oxide nanosheets: Properties, stability, and interconversion. Materials Letters, 2020, 275, 128067.	2.6	14
80	Theoretical study of MgO(001) surfaces: Pure, doped with Fe, Ca, and Al, and with and without adsorbed water. International Journal of Quantum Chemistry, 2001, 84, 705-713.	2.0	13
81	First-principles calculations and Raman scattering evidence for local symmetry lowering in rhombohedral ilmenite: temperature- and pressure-dependent studies. Journal of Physics Condensed Matter, 2018, 30, 485401.	1.8	13
82	Computational simulations of ZnO@GaN and GaN@ZnO core@shell nanotubes. Journal of Solid State Chemistry, 2018, 266, 217-225.	2.9	13
83	DFT study of Î±-alanine as a function of the medium polarity. Computational and Theoretical Chemistry, 2001, 544, 151-157.	1.5	12
84	Laser/Electron Irradiation on Indium Phosphide (InP) Semiconductor: Promising Pathways to In Situ Formation of Indium Nanoparticles. Particle and Particle Systems Characterization, 2018, 35, 1800237.	2.3	12
85	Experimental and theoretical interpretation of the order/disorder clusters in CeO2:La. Applied Surface Science, 2020, 510, 145216.	6.1	12
86	A new multifunctional two-dimensional monolayer based on silicon carbide. FlatChem, 2021, 30, 100286.	5.6	12
87	Propriedades eletrÃ´nicas, estruturais e constantes elÃ¡sticas do ZnO. Quimica Nova, 2010, 33, 810-815.	0.3	11
88	Controlling the Electronic, Structural, and Optical Properties of Novel MgTiO₃/LaNiO₃ Nanostructured Films for Enhanced Optoelectronic Devices. ACS Applied Nano Materials, 2019, 2, 2612-2620.	5.0	11
89	Experimental and Theoretical Insights into the Structural Disorder and Gas Sensing Properties of ZnO. ACS Applied Electronic Materials, 2021, 3, 1447-1457.	4.3	11
90	Pure and Ni2O3-decorated CeO2 nanoparticles applied as CO gas sensor: Experimental and theoretical insights. Ceramics International, 2022, 48, 14014-14025.	4.8	11

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91	Theoretical analysis on TiO2(110)/V surface. International Journal of Quantum Chemistry, 2001, 85, 44-51.	2.0	10
92	Towards an insight on photodamage in hair fibre by <scp>UV</scp>â€light: An experimental and theoretical study. International Journal of Cosmetic Science, 2013, 35, 539-545.	2.6	10
93	Choice of hybrid functional and basis set optimization to calculate the structural, electronic, mechanical, and vibrational properties of BaSnO3. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	10
94	4-Component correlated all-electron study on Eka-actinium Fluoride (E121F) including Gaunt interaction: Accurate analytical form, bonding and influence on rovibrational spectra. Chemical Physics Letters, 2016, 662, 169-175.	2.6	10
95	Piezoelectric Response of Porous Nanotubes Derived from Hexagonal Boron Nitride under Strain Influence. ACS Omega, 2018, 3, 13413-13421.	3.5	10
96	A quantum-mechanical investigation of oxygen vacancies and copper doping in the orthorhombic CaSnO₃ perovskite. Physical Chemistry Chemical Physics, 2018, 20, 20970-20980.	2.8	10
97	Surface and electronic properties of rutile TiO2 thin films coated with PbO2. Computational Materials Science, 2020, 171, 109222.	3.0	9
98	Morphological Transformation Network of Nanoparticles via DFT Simulations. Crystal Growth and Design, 2020, 20, 4600-4611.	3.0	9
99	Charge transfer in Pr-Doped cerium oxide: Experimental and theoretical investigations. Materials Chemistry and Physics, 2020, 249, 122967.	4.0	9
100	A promising carbon-based nanosheet as a suitable Na-anode material. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2021, 268, 115121.	3.5	9
101	Ab Initio correlated all electron Dirac-Fock calculations for eka-francium fluoride (E119F). Journal of the Brazilian Chemical Society, 2012, 23, 1104-1113.	0.6	9
102	NH3+N2O3 reaction. High level calculations. Computational and Theoretical Chemistry, 2006, 759, 189-194.	1.5	8
103	All electron fully relativistic Diracâ€“Fock calculation for darmstadtium carbide using prolapse free basis set. Chemical Physics Letters, 2007, 440, 367-371.	2.6	8
104	Structure, optical properties, and photocatalytic activity of Î±-Ag2W0.75Mo0.25O4. Materials Research Bulletin, 2020, 132, 111011.	5.2	8
105	Unveiling the Structural Behavior under Pressure of Filled M_{0.5}Co₄Sb₁₂ (M = K, Sr, La, Ce, and Yb) Thermoelectric Skutterudites. Inorganic Chemistry, 2021, 60, 7413-7421.	4.0	8
106	One- and two-dimensional structures based on gallium nitride. Journal of Solid State Chemistry, 2021, 303, 122513.	2.9	8
107	Enhanced Photocatalytic and Photoluminescence Properties Resulting from Type-I Band Alignment in the Zn2GeO4/g-C3N4 Nanocomposites. Catalysts, 2022, 12, 692.	3.5	8
108	DFT studies on PbO2 and binary PbO2/SnO2 thin films. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 136, 115037.	2.7	7

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109	Ab initio study and NMR analysis of the complexion of citric acid with ion lithium. Computational and Theoretical Chemistry, 1999, 493, 309-318.	1.5	6
110	A joint theoretical and kinetic investigation on the fragmentation of (N-halo)-2-amino cycloalkanecarboxylates. Chemical Physics, 2002, 280, 1-14.	1.9	6
111	AnÃ¡lise teÃ³rica da interaÃ§Ã£o de CO, CO2 e NH3 com ZnO. Quimica Nova, 2004, 27, 10-16.	0.3	6
112	Theoretical-experimental evaluation of the photocatalytic activity of KCa2Ta3â^'xNbxO10. Materials Letters, 2019, 253, 392-395.	2.6	6
113	Unveiling the infrared complex dielectric function of ilmenite CdTiO3. Journal of Alloys and Compounds, 2020, 813, 152136.	5.5	6
114	New 2D nanosheets based on the octa-graphene. Journal of Solid State Chemistry, 2020, 290, 121534.	2.9	6
115	Strain-induced novel properties of alloy nitride nanotubes. Computational Materials Science, 2020, 177, 109589.	3.0	6
116	Theoretical Study on Band Alignment Mechanism for the ZnO@ZnS Interface of Core-Shell Structures. Current Physical Chemistry, 2016, 5, 327-336.	0.2	6
117	Propriedades eletrÃ´nicas e estruturais do PbTiO3: teoria do funcional de densidade aplicada a modelos periÃ³dicos. Quimica Nova, 2005, 28, 10-18.	0.3	5
118	DFT study on the water-assisted mechanism for the reaction between VO+ and NH3 to yield VNH+ and H2O. Chemical Physics Letters, 2006, 427, 265-270.	2.6	5
119	Conducting Behavior of Crystalline Î±-PbO2 as Revealed by DFT Calculations. Materials Research, 2018, 21, .	1.3	5
120	New insights into the nature of the bandgap of CuGeO3 nanofibers: Synthesis, electronic structure, and optical and photocatalytic properties. Materials Today Communications, 2021, 26, 101701.	1.9	4
121	Unconventional Disorder by Femtosecond Laser Irradiation in Fe₂O₃. ACS Omega, 2021, 6, 28049-28062.	3.5	4
122	Efeitos da adiÃ§Ã£o de Ã¡tomos de Mn na rede do GaN via mÃ©todos de estrutura eletrÃ´nica. Quimica Nova, 2010, 33, 834-840.	0.3	3
123	Thermodynamic and electronic study of Ga1â^'xMnxN films. A theoretical study. Surface Science, 2011, 605, 1431-1437.	1.9	3
124	AlGaN double-walled nanotubes as ammonia gas sensor. Journal of Solid State Chemistry, 2020, 292, 121729.	2.9	3
125	Ab Initio Modeling of MultiWall: A General Algorithm First Applied to Carbon Nanotubes. Journal of Physical Chemistry A, 2021, 125, 4003-4012.	2.5	3
126	Piezoelectricity induced by gaseous molecules adsorbed on ZnO nanotubes. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2022, 281, 115729.	3.5	3

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127	First-principles Simulation of Elastic Constants and Electronic Properties of GaN. Current Physical Chemistry, 2014, 4, 65-70.	0.2	2
128	Optical phonon modes in 1:2 ordered trigonal Ba 3 MgNb 2 O 9 perovskite: Synergy of both classical and quantum methods. Journal of Raman Spectroscopy, 2020, 51, 1219-1229.	2.5	2
129	Intra-octahedral distortion on lamellar potassium niobate K₄Nb₆O₁₇: a periodic DFT study of structural, electronic and vibrational properties. Physical Chemistry Chemical Physics, 2020, 22, 16562-16570.	2.8	2
130	A promising nanoporous Al<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si29.svg"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math>Ga<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si30.svg"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mo		