

# Andrei N Enyashin

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

204  
papers

4,320  
citations

33  
h-index

60  
g-index

220  
ext. papers

4,835  
ext. citations

3.7  
avg, IF

5.79  
L-index

| #   | Paper   | IF   | Citations |
|-----|---|------|-----------|
| 204 | Synthesis and Structure of Quasi-One-Dimensional Niobium Tetrasulfide NbS <sub>4</sub> . <i>Inorganic Chemistry</i> , <b>2022</b> ,   | 5.1  | 1         |
| 203 | Nanotubes from the Misfit Layered Compound (SmS)TaS: Atomic Structure, Charge Transfer, and Electrical Properties.. <i>Chemistry of Materials</i> , <b>2022</b> , 34, 1838-1853   | 9.6  | 2         |
| 202 | Janus ZnS nanoparticles: Synthesis and photocatalytic properties. <i>Journal of Physics and Chemistry of Solids</i> , <b>2021</b> , 161, 110459   | 3.9  | 1         |
| 201 | V <sub>2</sub> O <sub>3</sub> /C composite fabricated by carboxylic acid-assisted sol-gel synthesis as anode material for lithium-ion batteries. <i>Journal of Sol-Gel Science and Technology</i> , <b>2021</b> , 98, 549-558                                       | 2.3  | 2         |
| 200 | First-principles study on the plutonium ions interaction with diamide molecules in acid solutions. <i>International Journal of Quantum Chemistry</i> , <b>2021</b> , 121, e26681  | 2.1  |           |
| 199 | Imogolite: Curvature-Induced Hospitality for Trivalent Dopants. <i>Physica Status Solidi (B): Basic Research</i> , <b>2021</b> , 258, 2100188   | 1.3  |           |
| 198 | Thermal and kinetic studies of sulfur-rich molybdenum and tungsten polysulfides. <i>Journal of Alloys and Compounds</i> , <b>2021</b> , 851, 156705   | 5.7  | 3         |
| 197 | Plutonium complexes in water: new approach to ab initio modeling. <i>Radiochimica Acta</i> , <b>2021</b> , 109, 327-342   |      | 1         |
| 196 | Asymmetric misfit nanotubes: Chemical affinity outwits the entropy at high-temperature solid-state reactions. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2021</b> , 118,   | 11.5 | 4         |
| 195 | Phase equilibrium within the composites of the cadmium sulfide nanoparticles and a silicate glass: An atomistic view. <i>Computational Materials Science</i> , <b>2021</b> , 199, 110726  | 3.2  |           |
| 194 | Structural and spectroscopic characterization of a new series of BaREGeO (RE = Pr, Nd, Gd, and Dy) and BaGdEuGeO tetragermanates. <i>Dalton Transactions</i> , <b>2021</b> , 50, 10935-10946  | 4.3  |           |
| 193 | Quaternary Ln <sub>x</sub> La <sub>(1-x)</sub> S-TaS <sub>2</sub> nanotubes (Ln=Pr, Sm, Ho, and Yb) as a vehicle for improving the yield of misfit nanotubes. <i>Applied Materials Today</i> , <b>2020</b> , 19, 100581   | 6.6  | 4         |
| 192 | YS-TaS and YLaS-TaS (0 <math>x</math> 1) Nanotubes: A Family of Misfit Layered Compounds. <i>ACS Nano</i> , <b>2020</b> , 14, 5445-5458   | 16.7 | 7         |
| 191 | Intrinsic defects and their influence on optical properties of Al <sub>9</sub> (GeO <sub>4</sub> ) <sub>6</sub> O <sub>2</sub> (Al = Li, Na, K, Rb, Cs) oxyapatites prepared by spray pyrolysis. <i>Journal of Alloys and Compounds</i> , <b>2020</b> , 839, 155609 | 5.7  | 1         |
| 190 | Nanostructured Pb(S, O) Films: Synthesis, Mechanism of Deposition, and Optical Properties. <i>Russian Journal of Physical Chemistry A</i> , <b>2020</b> , 94, 2421-2427   | 0.7  | 0         |
| 189 | NiWSe <sub>2</sub> nanostructures as efficient catalysts for electrochemical hydrogen evolution reaction (HER) in acidic and alkaline media. <i>Journal of Materials Chemistry A</i> , <b>2020</b> , 8, 1403-1416   | 13   | 43        |
| 188 | Synthesis, spectroscopic and luminescence properties of Ga-doped $\beta$ -AlO. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2020</b> , 227, 117658   | 4.4  | 6         |

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|-----|---|-----|----|
| 187 | Structural and chemical mechanism underlying formation of Zn <sub>2</sub> SiO <sub>4</sub> :Mn crystalline phosphor properties. <i>Journal of Alloys and Compounds</i> , <b>2020</b> , 820, 153129  | 5.7 | 6  |
| 186 | Local environment of CdS nanoparticles incorporated into anatase/brookite matrix via sol-gel route: HRTEM, Raman spectroscopy and MD simulation. <i>Materials Today Communications</i> , <b>2020</b> , 25, 101465   | 2.5 | 2  |
| 185 | Crystal structure, luminescence properties and thermal stability of BaY <sub>2</sub> EuGe <sub>3</sub> O <sub>10</sub> phosphors with high colour purity for blue-excited pc-LEDs. <i>New Journal of Chemistry</i> , <b>2020</b> , 44, 16400-16411                        | 3.6 | 5  |
| 184 | New phase within the SrO <sub>2</sub> BO <sub>3</sub> TeO <sub>2</sub> (R = Dy, Lu) systems: Synthesis and quantum-chemical modeling. <i>Journal of Physics and Chemistry of Solids</i> , <b>2020</b> , 138, 109241   | 3.9 |    |
| 183 | Photolysis of polychlorobiphenyls in the presence of nanocrystalline TiO <sub>2</sub> and CdS/TiO <sub>2</sub> . <i>Reaction Kinetics, Mechanisms and Catalysis</i> , <b>2019</b> , 126, 1115-1134  | 1.6 | 3  |
| 182 | Theoretical and experimental comparative study of the stability and phase transformations of sesquichalcogenides MQ (M = Nb, Mo; Q = S, Se). <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 1454-1463   | 3.6 | 8  |
| 181 | Low-Temperature Sol-Gel Synthesis and Photoactivity of Nanocrystalline TiO <sub>2</sub> with the Anatase/Brookite Structure and an Amorphous Component. <i>Kinetics and Catalysis</i> , <b>2019</b> , 60, 325-336   | 1.5 | 5  |
| 180 | Synthesis and characterization of quaternary La(Sr)S-TaS misfit-layered nanotubes. <i>Beilstein Journal of Nanotechnology</i> , <b>2019</b> , 10, 1112-1124   | 3   | 4  |
| 179 | Study of structural, spectroscopic and photo-oxidation properties of in-situ synthesized Sc-doped titania. <i>Journal of Molecular Liquids</i> , <b>2019</b> , 284, 29-38   | 6   | 1  |
| 178 | Ion sensor activity of BiMoO <sub>3</sub> prepared using microwave-assisted hydrothermal synthesis. <i>Journal of Electroanalytical Chemistry</i> , <b>2019</b> , 840, 187-192  | 4.1 | 5  |
| 177 | Understanding the formation thermodynamics of fresnoitic trivanadates: DFT calculations and soft base hydrolysis synthesis. <i>Journal of Physics and Chemistry of Solids</i> , <b>2019</b> , 124, 7-12   | 3.9 |    |
| 176 | Revealing the Flexible 1D Primary and Globular Secondary Structures of Sulfur-Rich Amorphous Transition Metal Polysulfides. <i>ChemNanoMat</i> , <b>2019</b> , 5, 1488-1497   | 3.5 | 4  |
| 175 | Electrochemical Oxidative Aromatization of 9-Substituted 9,10-Dihydroacridines: Cleavage of C-H vs C-C Bond. <i>Chemistry of Heterocyclic Compounds</i> , <b>2019</b> , 55, 956-963   | 1.4 | 3  |
| 174 | Structural, electronic, and optical studies of BaRE <sub>2</sub> Ge <sub>3</sub> O <sub>10</sub> (RE = Y, Sc, Gd, Lu) germanates with a special focus on the [Ge <sub>3</sub> O <sub>10</sub> ] <sup>8-</sup> geometry. <i>CrystEngComm</i> , <b>2019</b> , 21, 6491-6502 | 3.3 | 7  |
| 173 | Effect of Ru Doping on the Properties of MoSe <sub>2</sub> Nanoflowers. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 1987-1994   | 3.8 | 36 |
| 172 | Synthesis, crystal structure and optical properties of Me(OH)(HCOO) <sub>2</sub> (Me = Al, Ga). <i>CrystEngComm</i> , <b>2018</b> , 20, 2741-2748   | 3.3 | 6  |
| 171 | Structure, magnetic and optical properties of Sr <sub>3</sub> RE <sub>2</sub> (Ge <sub>3</sub> O <sub>9</sub> ) <sub>2</sub> cyclogermanates (RE = La, Lu). <i>CrystEngComm</i> , <b>2018</b> , 20, 2404-2412   | 3.3 | 4  |
| 170 | Sensitized IR luminescence in Ca <sub>3</sub> Y <sub>2</sub> Ge <sub>3</sub> O <sub>12</sub> : Nd <sup>3+</sup> , Ho <sup>3+</sup> under 808 nm laser excitation. <i>Ceramics International</i> , <b>2018</b> , 44, 6959-6967   | 5.1 | 13 |

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|-----|---|-----|----|
| 169 | Nitrogen-doped ZnS nanoparticles: Soft-chemical synthesis, EPR statement and quantum-chemical characterization. <i>Materials Chemistry and Physics</i> , <b>2018</b> , 215, 176-182   | 4.4 | 5  |
| 168 | Stability and electronic properties of oxygen-doped ZnS polytypes: DFTB study. <i>Chemical Physics</i> , <b>2018</b> , 510, 70-76   | 2.3 | 1  |
| 167 | Metal cations doped vanadium oxide nanotubes: Synthesis, electronic structure, and gas sensing properties. <i>Sensors and Actuators B: Chemical</i> , <b>2018</b> , 256, 1021-1029  | 8.5 | 14 |
| 166 | Concentration growth of luminescence intensity of phosphor Zn <sub>2-2x</sub> Mn <sub>2x</sub> SiO <sub>4</sub> (III.13): Crystal-chemical and quantum-mechanical justification. <i>Materials Research Bulletin</i> , <b>2018</b> , 97, 182-188 | 5.1 | 13 |
| 165 | Single Walled Bil Nanotubes Encapsulated within Carbon Nanotubes. <i>Scientific Reports</i> , <b>2018</b> , 8, 10133  | 4.9 | 6  |
| 164 | XPS experimental and DFT investigations on solid solutions of MoReS (0 Nanoscale, <b>2018</b> , 10, 10232-10240   | 7.9 | 17 |
| 163 | Titanium Dichalcogenides as Nanoreactors for Magnetic High-Anisotropy Phases. <i>Journal of Physical Chemistry Letters</i> , <b>2018</b> , 9, 5183-5188   | 6.4 | 0  |
| 162 | Polymorphism and properties of ammonium scandium sulfate (NH <sub>4</sub> ) <sub>3</sub> Sc(SO <sub>4</sub> ) <sub>3</sub> : new intermediate compound in scandium production. <i>CrystEngComm</i> , <b>2018</b> , 20, 3772-3783                | 3.3 | 3  |
| 161 | Capillary filling of carbon nanotubes by BiCl <sub>3</sub> : TEM and MD insight. <i>Nanosystems: Physics, Chemistry, Mathematics</i> , <b>2018</b> , 521-531  | 1.8 | 2  |
| 160 | Size dependent content of structural vacancies within TiO nanoparticles: Quantum-chemical DFTB study. <i>Superlattices and Microstructures</i> , <b>2018</b> , 113, 459-465   | 2.8 | 7  |
| 159 | An Xps Study of Solid Solutions Mo <sub>1-x</sub> Nb <sub>x</sub> S <sub>2</sub> (0 Journal of Structural Chemistry, <b>2018</b> , 59, 1833-1840  | 0.9 |    |
| 158 | Morphological Phase Diagram of Gadolinium Iodide Encapsulated in Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , <b>2018</b> , 122, 24967-24976  | 3.8 | 4  |
| 157 | Nd,Ho-Codoped apatite-related NaLa(GeO)O phosphors for the near- and middle-infrared region. <i>Dalton Transactions</i> , <b>2018</b> , 47, 14041-14051   | 4.3 | 5  |
| 156 | Cu <sub>2</sub> S/MoS <sub>2</sub> Nano-Octahedra at the Atomic Scale: Using a Template To Activate the Basal Plane of MoS <sub>2</sub> for Hydrogen Production. <i>Chemistry of Materials</i> , <b>2018</b> , 30, 4489-4492                    | 9.6 | 34 |
| 155 | Facile, rapid and efficient doping of amorphous TiO <sub>2</sub> by pre-synthesized colloidal CdS quantum dots. <i>Journal of Alloys and Compounds</i> , <b>2017</b> , 706, 205-214   | 5.7 | 9  |
| 154 | Quantum-chemical study of structural and electronic properties of a new tin monosulfide polymorph ESnS. <i>Doklady Physical Chemistry</i> , <b>2017</b> , 472, 23-26  | 0.8 | 1  |
| 153 | A DFT study and experimental evidence of the sonication-induced cleavage of molybdenum sulfide Mo <sub>2</sub> S <sub>3</sub> in liquids. <i>Journal of Materials Chemistry C</i> , <b>2017</b> , 5, 6601-6610                                  | 7.1 | 10 |
| 152 | Structure and Stability of GaS Fullerenes and Nanotubes. <i>Israel Journal of Chemistry</i> , <b>2017</b> , 57, 529-539   | 3.4 | 3  |

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|-----|--|------|----|
| 151 | Electronic structure and optical properties of $\text{ALa}_{9-x}\text{Eu}_x(\text{GeO}_4)_6\text{O}_2$ (A = Li, Na, K, Rb, Cs, La $^{1/3}$ ; x = 0, 0.07). <i>Journal of Alloys and Compounds</i> , <b>2017</b> , 727, 390-397       | 5.7  | 4  |
| 150 | Synthesis and crystal structure of 3R and 1T' polytypes of $\text{NH}_4\text{Sc}(\text{SO}_4)_2$ . <i>Journal of Solid State Chemistry</i> , <b>2017</b> , 255, 50-60  | 3.3  | 4  |
| 149 | Quantum-chemical study of titanium monoxide nanoparticles with structural vacancies. <i>Doklady Physical Chemistry</i> , <b>2017</b> , 473, 71-74  | 0.8  |    |
| 148 | Structural, electronic properties of microscale $(\text{NH}_4)_2\text{V}_3\text{O}_8$ fabricated using a novel preparation method. <i>Journal of Physics and Chemistry of Solids</i> , <b>2017</b> , 101, 58-64                      | 3.9  | 6  |
| 147 | Capillary Imbibition of Gadolinium Halides into WS $_2$ Nanotubes: a Molecular Dynamics View. <i>Israel Journal of Chemistry</i> , <b>2017</b> , 57, 501-508   | 3.4  | 0  |
| 146 | Structure and optical properties of $\text{KLa}_9(\text{GeO}_4)_6\text{O}_2$ and $\text{KLa}_{8.37}\text{Eu}_{0.63}(\text{GeO}_4)_6\text{O}_2$ . <i>Chemical Physics Letters</i> , <b>2017</b> , 667, 9-14                           | 2.5  | 6  |
| 145 | Diameter-dependent wetting of tungsten disulfide nanotubes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2016</b> , 113, 13624-13629  | 11.5 | 9  |
| 144 | Quantum-chemical study of quasi-one-dimensional vanadium and niobium sulfides with Peierls distortion. <i>Journal of Structural Chemistry</i> , <b>2016</b> , 57, 1505-1512  | 0.9  | 8  |
| 143 | Electronic structure and formation energies of nonstoichiometric dichalcogenides $\text{M}_x\text{X}_{2-x}$ (M = Nb, Mo, W; X = Se, Te). <i>Journal of Structural Chemistry</i> , <b>2016</b> , 57, 281-286                          | 0.9  | 1  |
| 142 | Structural and chemical analysis of gadolinium halides encapsulated within WS $_2$ nanotubes. <i>Nanoscale</i> , <b>2016</b> , 8, 12170-81   | 7.7  | 6  |
| 141 | Molecular dynamics simulations of defect formation in thin graphite films using the density functional tight-binding method. <i>Journal of Structural Chemistry</i> , <b>2016</b> , 57, 808-811                                      | 0.9  | 2  |
| 140 | A new polymorph of $\text{NH}_4\text{V}_3\text{O}_7$ : Synthesis, structure, magnetic and electrochemical properties. <i>Solid State Sciences</i> , <b>2016</b> , 61, 225-231  | 3.4  | 2  |
| 139 | Relative stability, electronic and structural properties in the family of $\text{NH}_4\text{V}_3\text{O}_7$ polymorphs from first principles calculations. <i>Computational and Theoretical Chemistry</i> , <b>2015</b> , 1070, 9-13 | 2    |    |
| 138 | Solar Synthesis of PbS-SnS $_2$ Superstructure Nanoparticles. <i>ACS Nano</i> , <b>2015</b> , 9, 7831-9  | 16.7 | 17 |
| 137 | Optical Properties of Triangular Molybdenum Disulfide Nanoflakes. <i>Journal of Physical Chemistry Letters</i> , <b>2014</b> , 5, 3636-40  | 6.4  | 26 |
| 136 | Atomic-scale evolution of a growing core-shell nanoparticle. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 12564-7  | 16.4 | 14 |
| 135 | Structural and electronic properties of new 1D and 2D carbon allotropes with mixed sp $^1$ & sp $^3$ hybridization types. <i>Chemical Physics Letters</i> , <b>2014</b> , 609, 15-20   | 2.5  | 2  |
| 134 | The Role of Lead (Pb) in the High Temperature Formation of MoS $_2$ Nanotubes. <i>Inorganics</i> , <b>2014</b> , 2, 363-376  | 3.6  | 5  |

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|-----|---|------|-----|
| 133 | On the capabilities of the x-ray diffraction method in determining polytypes in nanostructured layered metal disulfides. <i>Journal of Structural Chemistry</i> , <b>2013</b> , 54, 388-395   | 0.9  | 4   |
| 132 | Fluorographynes: Stability, structural and electronic properties. <i>Superlattices and Microstructures</i> , <b>2013</b> , 55, 75-82  | 2.8  | 21  |
| 131 | Structural, electronic, and elastic properties of Y-diamonds and their BN analogues. <i>Diamond and Related Materials</i> , <b>2013</b> , 38, 93-100  | 3.5  | 1   |
| 130 | Structural, electronic, mechanical, and magnetic properties and relative stability of polymorphic modifications of ReN <sub>2</sub> from Ab initio calculation data. <i>Physics of the Solid State</i> , <b>2013</b> , 55, 1821-1825  | 0.8  | 3   |
| 129 | Layers and tubes of fluorographene C <sub>4</sub> F: Stability, structural and electronic properties from DFTB calculations. <i>Chemical Physics Letters</i> , <b>2013</b> , 576, 44-48   | 2.5  | 11  |
| 128 | Two-dimensional titanium carbonitrides and their hydroxylated derivatives: Structural, electronic properties and stability of MXenes Ti <sub>3</sub> C <sub>2</sub> N <sub>x</sub> (OH) <sub>2</sub> from DFTB calculations. <i>Journal of Solid State Chemistry</i> , <b>2013</b> , 207, 42-48 | 3.3  | 103 |
| 127 | Line Defects in Molybdenum Disulfide Layers. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 10842-10848  | 3.8  | 105 |
| 126 | Structural and Electronic Properties and Stability of MXenes Ti <sub>2</sub> C and Ti <sub>3</sub> C <sub>2</sub> Functionalized by Methoxy Groups. <i>Journal of Physical Chemistry C</i> , <b>2013</b> , 117, 13637-13643   | 3.8  | 153 |
| 125 | Defect-induced conductivity anisotropy in MoS <sub>2</sub> monolayers. <i>Physical Review B</i> , <b>2013</b> , 88,   | 3.3  | 126 |
| 124 | Graphene-like transition-metal nanocarbides and nanonitrides. <i>Russian Chemical Reviews</i> , <b>2013</b> , 82, 735-746   | 3.6  | 60  |
| 123 | Stability and structural, elastic, and electronic properties of 3D-(sp <sup>3</sup> ) carbon allotropes according to DFTB calculations. <i>Doklady Physical Chemistry</i> , <b>2012</b> , 442, 1-4  | 0.8  | 5   |
| 122 | Controlled doping of MS <sub>2</sub> (M=W, Mo) nanotubes and fullerene-like nanoparticles. <i>Angewandte Chemie - International Edition</i> , <b>2012</b> , 51, 1148-51   | 16.4 | 67  |
| 121 | Fluorinated derivatives of sp <sup>2</sup> graphene allotropes: Structure, stability, and electronic properties. <i>Chemical Physics Letters</i> , <b>2012</b> , 545, 78-82   | 2.5  | 15  |
| 120 | Investigation of Rhenium-Doped MoS <sub>2</sub> Nanoparticles with Fullerene-Like Structure. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , <b>2012</b> , 638, 2610-2616   | 1.3  | 19  |
| 119 | On the crystallization of polymer composites with inorganic fullerene-like particles. <i>Physical Chemistry Chemical Physics</i> , <b>2012</b> , 14, 7104-11  | 3.6  | 4   |
| 118 | Atomic structure, comparative stability and electronic properties of hydroxylated Ti <sub>2</sub> C and Ti <sub>3</sub> C <sub>2</sub> nanotubes. <i>Computational and Theoretical Chemistry</i> , <b>2012</b> , 989, 27-32   | 2    | 120 |
| 117 | Diffraction from Disordered Stacking Sequences in MoS <sub>2</sub> and WS <sub>2</sub> Fullerenes and Nanotubes. <i>Journal of Physical Chemistry C</i> , <b>2012</b> , 116, 24350-24357  | 3.8  | 40  |
| 116 | Density-functional study of Li <sub>x</sub> MoS <sub>2</sub> intercalates (0 < x < 1). <i>Computational and Theoretical Chemistry</i> , <b>2012</b> , 999, 13-20  | 2    | 101 |

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|-----|---|------|-----|
| 115 | Atomic structure, stability and electronic properties of fluorinated diamond-like carbon nanolayers. <i>Theoretical and Experimental Chemistry</i> , <b>2012</b> , 48, 327-330  | 1.3  | 1   |
| 114 | Transport properties of MoS <sub>2</sub> nanoribbons: edge priority. <i>European Physical Journal B</i> , <b>2012</b> , 85, 1   | 1.2  | 53  |
| 113 | Do cement nanotubes exist?. <i>Advanced Materials</i> , <b>2012</b> , 24, 3239-45   | 24   | 37  |
| 112 | Controlled Doping of MS <sub>2</sub> (M=W, Mo) Nanotubes and Fullerene-like Nanoparticles. <i>Angewandte Chemie</i> , <b>2012</b> , 124, 1174-1177  | 3.6  | 2   |
| 111 | New Route for Stabilization of 1T-WS <sub>2</sub> and MoS <sub>2</sub> Phases. <i>Journal of Physical Chemistry C</i> , <b>2011</b> , 115, 24586-24596  | 3.6  | 2   |
| 110 | Nanotubes of layered iron-based superconductors: Simulations of atomic structure and electronic properties. <i>Computational Materials Science</i> , <b>2011</b> , 50, 824-827  | 3.2  | 3   |
| 109 | Composition, stability, and elastic moduli of higher allotropes of boron (EB and tII-B) according to SCC-DFTB calculations. <i>Doklady Physical Chemistry</i> , <b>2011</b> , 438, 118-121  | 0.8  |     |
| 108 | Modeling of the electronic structure, chemical bonding, and properties of ternary silicon carbide Ti <sub>3</sub> SiC <sub>2</sub> . <i>Journal of Structural Chemistry</i> , <b>2011</b> , 52, 785-802   | 0.9  | 47  |
| 107 | Structural, elastic, and electronic properties of icosahedral boron subcarbides (B <sub>12</sub> C <sub>3</sub> , B <sub>13</sub> C <sub>2</sub> ), subnitride B <sub>12</sub> N <sub>2</sub> , and suboxide B <sub>12</sub> O <sub>2</sub> from data of SCC-DFTB calculations. <i>Physics of the Solid State</i> , <b>2011</b> , 53, 1569-1574 | 0.8  | 9   |
| 106 | 3D Polymorphs of boron nitride: SCC-DFTB modeling of the stability and structural, elastic, and electronic characteristics. <i>Theoretical and Experimental Chemistry</i> , <b>2011</b> , 47, 155-158   | 1.3  | 3   |
| 105 | Graphene allotropes. <i>Physica Status Solidi (B): Basic Research</i> , <b>2011</b> , 248, 1879-1883  | 1.3  | 301 |
| 104 | MoS <sub>2</sub> Hybrid Nanostructures: From Octahedral to Quasi-Spherical Shells within Individual Nanoparticles. <i>Angewandte Chemie</i> , <b>2011</b> , 123, 1850-1854  | 3.6  | 8   |
| 103 | Inside Cover: MoS <sub>2</sub> Hybrid Nanostructures: From Octahedral to Quasi-Spherical Shells within Individual Nanoparticles (Angew. Chem. Int. Ed. 8/2011). <i>Angewandte Chemie - International Edition</i> , <b>2011</b> , 50, 1728-1728  | 16.4 |     |
| 102 | MoS <sub>2</sub> hybrid nanostructures: from octahedral to quasi-spherical shells within individual nanoparticles. <i>Angewandte Chemie - International Edition</i> , <b>2011</b> , 50, 1810-4  | 16.4 | 56  |
| 101 | Graphene-like BN allotropes: Structural and electronic properties from DFTB calculations. <i>Chemical Physics Letters</i> , <b>2011</b> , 509, 143-147  | 2.5  | 22  |
| 100 | Radial compression studies of WS <sub>2</sub> nanotubes in the elastic regime. <i>Journal of Vacuum Science and Technology B: Nanotechnology and Microelectronics</i> , <b>2011</b> , 29, 021009  | 1.3  | 17  |
| 99  | Adsorption of nucleotides on the rutile (110) surface. <i>International Journal of Materials Research</i> , <b>2010</b> , 101, 758-764  | 0.5  | 18  |
| 98  | Hollow V <sub>2</sub> O <sub>5</sub> nanoparticles (fullerene-like analogues) prepared by laser ablation. <i>Journal of the American Chemical Society</i> , <b>2010</b> , 132, 11214-22   | 16.4 | 43  |

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| 97 | Magnetic properties of NiCl <sub>2</sub> nanostructures. <i>Computational Materials Science</i> , <b>2010</b> , 49, 782-786  | 3.2  | 2   |
| 96 | Stability and Electronic Properties of Bismuth Nanotubes. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 22092-22097  | 3.8  | 27  |
| 95 | Structural, Electronic, and Mechanical Properties of Single-Walled Halloysite Nanotube Models. <i>Journal of Physical Chemistry C</i> , <b>2010</b> , 114, 11358-11363   | 3.8  | 196 |
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