# Eva Scholtzova

List of Publications by Year
in descending order



| 46 | 502 | 687363 13 | 677142 22 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 46 | 46 | 46 | 533 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Structural and spectroscopic characterization of ettringite mineral â€“combined DFT and experimental study. Journal of Molecular Structure, 2015, 1100, 215-224. | 3.6 | 59 |
| 2 | Influence of Synthesis Conditions on the Formation of a Kaolinitemethanol Complex and Simulation of its Vibrational Spectra. Clays and Clay Minerals, 2012, 60, 227-239. | 1.3 | 46 |
| 3 | Theoretical and experimental study of montmorillonite intercalated with tetramethylammonium cation. Vibrational Spectroscopy, 2013, 66, 123-131. | 2.2 | 42 |
| 4 | The combined inelastic neutron scattering and solid state DFT study of hydrogen atoms dynamics in a highly ordered kaolinite. Physics and Chemistry of Minerals, 2010, 37, 571-579. | 0.8 | 33 |
| 5 | Mechanical properties of ettringite and thaumasiteâ€”DFT and experimental study. Cement and Concrete Research, 2015, 77, 9-15. | 11.0 | 29 |
| 6 | Theoretical study of cation substitution in trioctahedral sheet of phyllosilicates. An effect on inner OH group. Computational and Theoretical Chemistry, 2003, 620, 1-8. | 1.5 | 23 |
| 7 | B3LYP/6-311++Gâ—â— study of structure and spinâ€“spin coupling constant in heparin disaccharide. Carbohydrate Research, 2007, 342, 1350-1356. | 2.3 | 23 |
| 8 | A model study of dickite intercalated with formamide and N-methylformamide. Physics and Chemistry of Minerals, 2008, 35, 299-309. | 0.8 | 22 |
| 9 | Hydrogen Bonding and Vibrational Spectra in Kaolinite-Dimethylsulfoxide and -Dimethylselenoxide Intercalatesâ€“A Solid-State Computational Study. Clays and Clay Minerals, 2009, 57, 54-71. | 1.3 | 20 |
| 10 | Experimental and computational study of thaumasite structure. Cement and Concrete Research, 2014, 59, 66-72. | 11.0 | 20 |
| 11 | Prediction of mechanical properties of grafted kaolinite â€“ A DFT study. Applied Clay Science, 2020, 193, 105692. | 5.2 | 19 |
| 12 | Structural and Spectroscopic Characterization of Montmorillonite Intercalated with N-Butylammonium Cations (N = 1-4) â€” Modeling and Experimental Study. Clays and Clay Minerals, 2016, 64, 401-412. | 1.3 | 19 |
| 13 | Structural properties of montmorillonite intercalated with tetraalkylammonium cationsâ€”Computational and experimental study. Vibrational Spectroscopy, 2014, 74, 120-126. | 2.2 | 17 |
| 14 | Ab initio structure determination of 5-anilinomethylene-2,2-dimethyl-1,3-dioxane-4,6-dione from laboratory powder data â€“ a combined use of X-ray, molecular and solid-state DFT study. Acta Crystallographica Section B: Structural Science, 2007, 63, 477-484. | 1.8 | 11 |
| 15 | Density functional theory study of the stability of the tetrabutylphosphonium and tetrabutylammonium montmorillonites. Clay Minerals, 2019, 54, 41-48. | 0.6 | 11 |
| 16 | Crystal and electronic structure of aqua(N-salicylidene-methylester-l-glutamato)Cu(II) monohydrate. Zeitschrift Fur Kristallographie - Crystalline Materials, 2004, 219, 112-116. | 0.8 | 11 |
| 17 | Stability of Tetrabutylphosphonium Beidellite Organoclay. Journal of Physical Chemistry C, 2018, 122, 8380-8389. | 3.1 | 10 |
| 18 | On local structural changes in lizardite-1T: {Si4+/Al3+}, {Si4+/Fe3+}, [Mg2+/Al3+], [Mg2+/Fe3+] substitutions. Physics and Chemistry of Minerals, 2005, 32, 362-373. | 0.8 | 9 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | A Precursor Approach for the Development of Lace-like Fe<sub>2</sub>O<sub>3</sub> Nanocrystallites Triggered by Pressure Dependent Nucleation and Growth of Akaganeite over Clay Based Composites for Toluene Combustion. Journal of Physical Chemistry C, 2019, 123, 26236-26250. | 3.1 | 9 |
| 20 | Preparation, characterization and adsorption properties of tetraalkylphosphonium organobeidellites. Applied Clay Science, 2021, 204, 105989. | 5.2 | 7 |
| 21 | Stability of Atrazineâ€“Smectite Intercalates: Density Functional Theory and Experimental Study. Minerals (Basel, Switzerland), 2021, 11, 554. | 2.0 | 7 |
| 22 | (1-Methylimidazole)(N-salicylidene-rac-glutamato)copper(II). Acta Crystallographica Section E: Structure Reports Online, 2003, 59, m1181-m1183. | 0.2 | 6 |
| 23 | Ab initio 2-D periodic Hartree-Fock study of Fe-substituted lizardite 1 T - a simplified cronstedtite model. Physics and Chemistry of Minerals, 2000, 27, 741-746. | 0.8 | 5 |
| 24 | Modeling of Nontraditional Structures of Carbon. Journal of Chemical Information and Computer Sciences, 2001, 41, 451-456. | 2.8 | 5 |
| 25 | Structure of Sulfated Monosaccharides Studied by Quantum Chemical Methods. Molecules, 2003, 8, 770-779. | 3.8 | 5 |
| 26 | (N-Salicylidene-D,L-glutamato)(2-methylimidazole)copper(II). Acta Crystallographica Section E: Structure Reports Online, 2004, 60, m129-m132. | 0.2 | 5 |
| 27 | Time-of-flight Rietveld neutron structure refinement and quantum chemistry study of Y-Î±-sialon. Journal of the European Ceramic Society, 2006, 26, 3925-3931. | 5.7 | 5 |
| 28 | Combined powder diffraction and solid-state DFT study of [Cu (2,6-dimethoxynicotinate)2(Î¼-ronicol)2]n complex. Zeitschrift Fur Kristallographie - Crystalline Materials, 2008, 223, . | 0.8 | 5 |
| 29 | 2-(4-Hydroxyphenyl)-4,4-dimethyl-2-oxazoline: X-ray and density functional theory study. Acta Crystallographica Section C: Crystal Structure Communications, 2006, 62, o416-o418. | 0.4 | 2 |
| 30 | 3-(4-Bromophenyl)-5-(4-dimethylaminophenyl)-1-phenyl-2-pyrazoline: X-ray and density functional theory (DFT) studies. Acta Crystallographica Section C: Crystal Structure Communications, 2007, 63, o340-o342. | 0.4 | 2 |
| 31 | Crystal Structure, Infrared Spectra and DFT Study of Benzyl 2,3-Anhydro-Î²-d-Ribopyranoside. Journal of Chemical Crystallography, 2011, 41, 167-174. | 1.1 | 2 |
| 32 | DFT study of Rb-TFA structure after high-pressure action. Physics and Chemistry of Minerals, 2011, 38, 819-824. | 0.8 | 2 |
| 33 | Computational modeling of nanoclays. , 2020, , 139-166. | | 2 |
| 34 | Insight into the Structure of TMA-Hectorite: A Theoretical Approach. Minerals (Basel, Switzerland), 2021, 11, 505. | 2.0 | 2 |
| 35 | On recognition of FA/NMFA-dickite intercalates â€“ total energyvsintensity data. Acta Crystallographica Section A: Foundations and Advances, 2007, 63, s272-s273. | 0.3 | 2 |
| 36 | NBO analysis - a useful tool on interpretation of results of crystal structure determination. Acta Crystallographica Section A: Foundations and Advances, 2009, 65, s270-s270. | 0.3 | 2 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | 2-Anilinomethylene-3-oxobutanenitrile: an X-ray and density functional theory study. Acta Crystallographica Section C: Crystal Structure Communications, 2006, 62, o544-o546. | 0.4 | 1 |
| 38 | (E)-Methyl 2-anilinomethylene-3-oxobutanoate: X-ray and density functional theory studies. Acta Crystallographica Section C: Crystal Structure Communications, 2007, 63, o552-o554. | 0.4 | 1 |
| 39 | Powder diffraction and solid state DFT study of thetrans-bis(5-methylsalicylato)-bis(N,N-diethylnicotinamide)-diaquacopper(II) complex structure. Zeitschrift FÄ¼r Kristallographie, 2011, 226, 756-761. | 1.1 | 1 |
| 40 | Structural aspects of some CuIIcomplexes containing Schiff base. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, s266-s266. | 0.3 | 0 |
| 41 | anti-2-Hydroxy-2-methyl-1-tetralone oxime: X-ray and density functional theory study. Acta Crystallographica Section C: Crystal Structure Communications, 2006, 62, o199-o202. | 0.4 | 0 |
| 42 | 2-(2-Oxazolin-2-yl)benzene-1,4-diol: X-ray and density functional theory studies. Acta Crystallographica Section C: Crystal Structure Communications, 2007, 63, o187-o189. | 0.4 | 0 |
| 43 | Model Study of Partial Structural Decomposition of Thaumasite. Applied Mechanics and Materials, 2015, 749, 8-12. | 0.2 | 0 |
| 44 | Crystal and electronic structure of aqua(N-salicylidene-methylester-<scp>L</scp>-glutamato)Cu(II) monohydrate. Acta Crystallographica Section A: Foundations and Advances, 2002, 58, c133-c133. | 0.3 | 0 |
| 45 | On hydrogen bonding in DMSO and DMSeO â€“ kaolinite intercalates. Acta Crystallographica Section A: Foundations and Advances, 2007, 63, s273-s273. | 0.3 | 0 |
| 46 | Immobilisation of diuron herbicide employing smectites. Materials Today Communications, 2022, 31, 103252. | 1.9 | 0 |