

Eva Scholtzova

List of Publications by Year in descending order

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citing authors

#	ARTICLE	IF	CITATIONS
1	Immobilisation of diuron herbicide employing smectites. Materials Today Communications, 2022, 31, 103252.	1.9	0
2	Preparation, characterization and adsorption properties of tetraalkylphosphonium organobeidellites. Applied Clay Science, 2021, 204, 105989.	5.2	7
3	Stability of Atrazine-“Smectite Intercalates: Density Functional Theory and Experimental Study. Minerals (Basel, Switzerland), 2021, 11, 554.	2.0	7
4	Insight into the Structure of TMA-Hectorite: A Theoretical Approach. Minerals (Basel, Switzerland), 2021, 11, 505.	2.0	2
5	Prediction of mechanical properties of grafted kaolinite – A DFT study. Applied Clay Science, 2020, 193, 105692.	5.2	19
6	Computational modeling of nanoclays., 2020, , 139-166.		2
7	A Precursor Approach for the Development of Lace-like Fe ₂ O ₃ 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
8	Density functional theory study of the stability of the tetrabutylphosphonium and tetrabutylammonium montmorillonites. Clay Minerals, 2019, 54, 41-48.	0.6	11
9	Stability of Tetrabutylphosphonium Beidellite Organoclay. Journal of Physical Chemistry C, 2018, 122, 8380-8389.	3.1	10
10	Structural and Spectroscopic Characterization of Montmorillonite Intercalated with <i><sub>i</sub>N<sub>i</sub></i> -Butylammonium Cations (<i><sub>i</sub>N<sub>i</sub></i> = 1-4) – Modeling and Experimental Study. Clays and Clay Minerals, 2016, 64, 401-412.	1.3	19
11	Model Study of Partial Structural Decomposition of Thaumasite. Applied Mechanics and Materials, 2015, 749, 8-12.	0.2	0
12	Structural and spectroscopic characterization of ettringite mineral – combined DFT and experimental study. Journal of Molecular Structure, 2015, 1100, 215-224.	3.6	59
13	Mechanical properties of ettringite and thaumasite–DFT and experimental study. Cement and Concrete Research, 2015, 77, 9-15.	11.0	29
14	Experimental and computational study of thaumasite structure. Cement and Concrete Research, 2014, 59, 66-72.	11.0	20
15	Structural properties of montmorillonite intercalated with tetraalkylammonium cations–Computational and experimental study. Vibrational Spectroscopy, 2014, 74, 120-126.	2.2	17
16	Theoretical and experimental study of montmorillonite intercalated with tetramethylammonium cation. Vibrational Spectroscopy, 2013, 66, 123-131.	2.2	42
17	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
18	Powder diffraction and solid state DFT study of the trans-bis(5-methylsalicylato)-bis(N,N-diethylnicotinamide)-diaquacopper(II) complex structure. Zeitschrift für Kristallographie, 2011, 226, 756-761.	1.1	1

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19	Crystal Structure, Infrared Spectra and DFT Study of Benzyl 2,3-Anhydro- β -D-Ribopyranoside. <i>Journal of Chemical Crystallography</i> , 2011, 41, 167-174.	1.1	2
20	DFT study of Rb-TFA structure after high-pressure action. <i>Physics and Chemistry of Minerals</i> , 2011, 38, 819-824.	0.8	2
21	The combined inelastic neutron scattering and solid state DFT study of hydrogen atoms dynamics in a highly ordered kaolinite. <i>Physics and Chemistry of Minerals</i> , 2010, 37, 571-579.	0.8	33
22	Hydrogen Bonding and Vibrational Spectra in Kaolinite-Dimethylsulfoxide and -Dimethylselenoxide Intercalates—A Solid-State Computational Study. <i>Clays and Clay Minerals</i> , 2009, 57, 54-71.	1.3	20
23	NBO analysis - a useful tool on interpretation of results of crystal structure determination. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2009, 65, s270-s270.	0.3	2
24	A model study of dickite intercalated with formamide and N-methylformamide. <i>Physics and Chemistry of Minerals</i> , 2008, 35, 299-309.	0.8	22
25	Combined powder diffraction and solid-state DFT study of [Cu (2,6-dimethoxynicotinate) ₂ ($\text{H}_4\text{-ronicol}$) ₂] _n complex. <i>Zeitschrift Fur Kristallographie - Crystalline Materials</i> , 2008, 223, .	0.8	5
26	2-(2-Oxazolin-2-yl)benzene-1,4-diol: X-ray and density functional theory studies. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2007, 63, o187-o189.	0.4	0
27	3-(4-Bromophenyl)-5-(4-dimethylaminophenyl)-1-phenyl-2-pyrazoline: X-ray and density functional theory (DFT) studies. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2007, 63, o340-o342.	0.4	2
28	(E)-Methyl 2-anilinomethylene-3-oxobutanoate: X-ray and density functional theory studies. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2007, 63, o552-o554.	0.4	1
29	Ab initio structure determination of 5-anilinomethylene-2,2-dimethyl-1,3-dioxane-4,6-dione from laboratory powder data – a combined use of X-ray, molecular and solid-state DFT study. <i>Acta Crystallographica Section B: Structural Science</i> , 2007, 63, 477-484.	1.8	11
30	B3LYP/6-311++G $\ddot{\text{a}}\text{-}\ddot{\text{a}}$ — study of structure and spin–spin coupling constant in heparin disaccharide. <i>Carbohydrate Research</i> , 2007, 342, 1350-1356.	2.3	23
31	On recognition of FA/NMFA-dickite intercalates – total energy vs intensity data. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2007, 63, s272-s273.	0.3	2
32	On hydrogen bonding in DMSO and DMSeO – kaolinite intercalates. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2007, 63, s273-s273.	0.3	0
33	anti-2-Hydroxy-2-methyl-1-tetralone oxime: X-ray and density functional theory study. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2006, 62, o199-o202.	0.4	0
34	2-(4-Hydroxyphenyl)-4,4-dimethyl-2-oxazoline: X-ray and density functional theory study. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2006, 62, o416-o418.	0.4	2
35	2-Anilinomethylene-3-oxobutanenitrile: an X-ray and density functional theory study. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2006, 62, o544-o546.	0.4	1
36	Time-of-flight Rietveld neutron structure refinement and quantum chemistry study of Y- f -sialon. <i>Journal of the European Ceramic Society</i> , 2006, 26, 3925-3931.	5.7	5

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37	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
38	(N-Salicylidene-D,L-glutamato)(2-methylimidazole)copper(II). Acta Crystallographica Section E: Structure Reports Online, 2004, 60, m129-m132.	0.2	5
39	Structural aspects of some Cullcomplexes containing Schiff base. Acta Crystallographica Section A: Foundations and Advances, 2004, 60, s266-s266.	0.3	0
40	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
41	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
42	(1-Methylimidazole)(N-salicylidene-rac-glutamato)copper(II). Acta Crystallographica Section E: Structure Reports Online, 2003, 59, m1181-m1183.	0.2	6
43	Structure of Sulfated Monosaccharides Studied by Quantum Chemical Methods. Molecules, 2003, 8, 770-779.	3.8	5
44	Crystal and electronic structure of aqua(<i>N</i>-salicylidene-methylester-<scp>L</scp>-glutamato)Cu(II) monohydrate. Acta Crystallographica Section A: Foundations and Advances, 2002, 58, c133-c133.	0.3	0
45	Modeling of Nontraditional Structures of Carbon. Journal of Chemical Information and Computer Sciences, 2001, 41, 451-456.	2.8	5
46	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