Kacper DruÅ¼bicki

List of Publications by Year
in descending order

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35 papers	509 citations	623734 14 h-index	713466 21 g-index
37 all docs	37 docs citations	37 times ranked	657 citing authors

#	Article	IF	Citations
1	Along the road to crystal structure prediction (CSP) of pharmaceutical-like molecules. CrystEngComm, 2022, 24, 1665-1678.	2.6	11
2	Cation Dynamics and Structural Stabilization in Formamidinium Lead Iodide Perovskites. Journal of Physical Chemistry Letters, 2021, 12, 3503-3508.	4.6	22
3	Dynamics & Spectroscopy with Neutronsâ€"Recent Developments & Emerging Opportunities. Polymers, 2021, 13, 1440.	4.5	8
4	Mapping of Guest Localization in Mesoporous Silica Particles by Solid-State NMR and Ab Initio Modeling: New Insights into Benzoic Acid and p-Fluorobenzoic Acid Embedded in MCM-41 via Ball Milling. Journal of Physical Chemistry C, 2021, 125, 10096-10109.	3.1	16
5	Interplay between Local Structure and Nuclear Dynamics in Tungstic Acid: A Neutron Scattering Study. Journal of Physical Chemistry C, 2021, 125, 23864-23879.	3.1	4
6	Spectroscopic Signatures of Hydrogen-Bonding Motifs in Protonic Ionic Liquid Systems: Insights from Diethylammonium Nitrate in the Solid State. Journal of Physical Chemistry C, 2021, 125, 24463-24476.	3.1	4
7	Vibrational Response of Felodipine in the THz Domain: Optical and Neutron Spectroscopy Versus Plane-Wave DFT Modeling. Journal of Infrared, Millimeter, and Terahertz Waves, 2020, 41, 1301-1336.	2.2	7
8	In silico Raman spectroscopy of YAlO3 single-crystalline film. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 231, 118111.	3.9	7
9	Environmental Effects on the Molecular Mobility of Ranitidine Hydrochloride: Crystalline State versus Drug Loaded into the Silica Matrix. Journal of Physical Chemistry C, 2019, 123, 18364-18375.	3.1	10
10	Diversity of methyl group dynamics in felodipine: a DFT supported NMR and QENS study. CrystEngComm, 2018, 20, 7371-7385.	2.6	8
11	Elucidating the Structure of Ranitidine Hydrochloride Form II: Insights from Solid-State Spectroscopy and Ab Initio Simulations. Crystal Growth and Design, 2018, 18, 4671-4681.	3.0	10
12	Molecular dynamics and the dissolution rate of nifedipine encapsulated in mesoporous silica. Microporous and Mesoporous Materials, 2017, 250, 186-194.	4.4	12
13	Molecular and Vibrational Dynamics in the Cholesterol-Lowering Agent Lovastatin: Solid-State NMR, Inelastic Neutron Scattering, and Periodic DFT Study. Journal of Physical Chemistry B, 2017, 121, 2776-2787.	2.6	15
14	Nuclear dynamics and phase polymorphism in solid formic acid. Physical Chemistry Chemical Physics, 2017, 19, 9064-9074.	2.8	33
15	Structureâ€"Spectra Correlations in Anilate Complexes with Picolines. Crystal Growth and Design, 2016, 16, 6069-6083.	3.0	3
16	On the molecular dynamics in long-acting calcium channel blocker lacidipine: solid-state NMR, neutron scattering and periodic DFT study. RSC Advances, 2016, 6, 66617-66629.	3.6	3
17	Unexpected Cation Dynamics in the Low-Temperature Phase of Methylammonium Lead Iodide: The Need for Improved Models. Journal of Physical Chemistry Letters, 2016, 7, 4701-4709.	4.6	53
18	In search of the mutual relationship between the structure, solid-state spectroscopy and molecular dynamics in selected calcium channel blockers. European Journal of Pharmaceutical Sciences, 2016, 85, 68-83.	4.0	16

#	Article	IF	Citations
19	Experimental (X-ray, ¹³C CP/MAS NMR, IR, RS, INS, THz) and Solid-State DFT Study on (1:1) Co-Crystal of Bromanilic Acid and 2,6-Dimethylpyrazine. Journal of Physical Chemistry B, 2015, 119, 6852-6872.	2.6	18
20	On the relaxation dynamics in active pharmaceutical ingredients: solid-state 1H NMR, quasi-elastic neutron scattering and periodic DFT study of acebutolol hydrochloride. RSC Advances, 2015, 5, 57502-57514.	3.6	4
21	Polymorphism of Resorcinol Explored by Complementary Vibrational Spectroscopy (FT-RS, THz-TDS,) Tj ETQq1 1 0.784314 rgBT /Over 2015, 119, 1681-1695.	2.6	35
22	Computationally Supported Neutron Scattering Study of Parent and Chemically Reduced Graphene Oxide. Journal of Physical Chemistry C, 2015, 119, 18650-18662.	3.1	17
23	Mesoporous drug carrier systems for enhanced delivery rate of poorly water-soluble drug: nimodipine. Journal of Porous Materials, 2015, 22, 817-829.	2.6	30
24	Computationally Assisted (Solid-State Density Functional Theory) Structural (X-ray) and Vibrational Spectroscopy (FT-IR, FT-RS, TDs-THz) Characterization of the Cardiovascular Drug Lacidipine. Crystal Growth and Design, 2015, 15, 2817-2830.	3.0	21
25	Nuclear dynamics in the metastable phase of the solid acid caesium hydrogen sulfate. Physical Chemistry Chemical Physics, 2015, 17, 31287-31296.	2.8	33
26	A comprehensive study on crystal structure, thermal behavior, and molecular dynamics of [Sr(DMSO)₄(NO₃)₂]. Journal of Coordination Chemistry, 2014, 67, 3135-3154.	2.2	5
27	Complementary optical and neutron vibrational spectroscopy study of bromanilic acid: 2,3,5,6-tetramethylpyrazine (1:1) cocrystal. Vibrational Spectroscopy, 2014, 75, 26-38.	2.2	12
28	Vibrational properties of water retained in graphene oxide. Chemical Physics Letters, 2014, 600, 106-111.	2.6	7
29	Experimental and Solid-State Computational Study of Structural and Dynamic Properties in the Equilibrium Form of Temazepam. Journal of Physical Chemistry B, 2014, 118, 6670-6679.	2.6	5
30	Solid-state DFT-assisted Raman study of titaniate nanostructures. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 116, 646-650.	3.9	13
31	Dynamics and the mesomorphic properties of a novel antiferroelectric liquid crystalline thiobenzoate MHPSBO10: Thermal, optical and dielectric spectroscopy study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2013, 105, 424-438.	3.9	1
32	Temperature-Dependent Infrared Spectroscopy Studies of a Novel Antiferroelectric Liquid-Crystalline Thiobenzoate. Journal of Physical Chemistry B, 2012, 116, 11332-11343.	2.6	5
33	Complex Vibrational Analysis of an Antiferroelectric Liquid Crystal Based on Solid-State Oriented Quantum Chemical Calculations and Experimental Molecular Spectroscopy. Journal of Physical Chemistry A, 2012, 116, 7809-7821.	2.5	10
34	Molecular structure and vibrational spectrum of [Mg((CH3)2SO)6](ClO4)2 studied by infrared and Raman spectroscopies and DFT computations. Journal of Molecular Structure, 2010, 970, 139-146.	3.6	22
35	Experimental (FT-IR, FT-RS) and theoretical (DFT) studies of vibrational dynamics and molecular structure of 4-n-pentylphenyl-4â€²-n-octyloxythiobenzoate (8OS5). Vibrational Spectroscopy, 2010, 52, 54-62.	2.2	29