Jefferson Maul

List of Publications by Year
in descending order

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27 papers	640 citations	430754 18 h-index	580701 25 g-index
27 all docs	27 docs citations	27 times ranked	799 citing authors

#	Article	IF	Citations
1	Thermal properties of molecular crystals through dispersion-corrected quasi-harmonic ab initio calculations: the case of urea. Chemical Communications, 2016, 52, 1820-1823.	2.2	65
2	Assessing thermochemical properties of materials through ab initio quantum-mechanical methods: the case of Î±-Al₂O₃. Physical Chemistry Chemical Physics, 2015, 17, 11670-11677.	1.3	51
3	Black and green pigments based on chromiumâ€“cobalt spinels. Materials Chemistry and Physics, 2011, 129, 619-624.	2.0	48
4	Probing the Mechanochemistry of Metalâ€“Organic Frameworks with Low-Frequency Vibrational Spectroscopy. Journal of Physical Chemistry C, 2018, 122, 27442-27450.	1.5	37
5	Anharmonic Vibrational States of Solids from DFT Calculations. Part II: Implementation of the VSCF and VCI Methods. Journal of Chemical Theory and Computation, 2019, 15, 3766-3777.	2.3	37
6	Structural and elastic anisotropy of crystals at high pressures and temperatures from quantum mechanical methods: The case of Mg2SiO4 forsterite. Journal of Chemical Physics, 2015, 142, 204502.	1.2	36
7	Anharmonic Vibrational States of Solids from DFT Calculations. Part I: Description of the Potential Energy Surface. Journal of Chemical Theory and Computation, 2019, 15, 3755-3765.	2.3	36
8	TiO2 synthesized by microwave assisted solvothermal method: Experimental and theoretical evaluation. Journal of Solid State Chemistry, 2014, 210, 171-177.	1.4	34
9	Anharmonic Thermal Oscillations of the Electron Momentum Distribution in Lithium Fluoride. Physical Review Letters, 2015, 115, 117402.	2.9	30
10	In silico infrared and Raman spectroscopy under pressure: The case of CaSnO3 perovskite. Journal of Chemical Physics, 2015, 142, 014505.	1.2	28
11	Pressure-driven mechanical anisotropy and destabilization in zeolitic imidazolate frameworks. Physical Review B, 2019, 99, .	1.1	27
12	Calculation of the Infrared Intensity of Crystalline Systems. A Comparison of Three Strategies Based on Berry Phase, Wannier Function, and Coupled-Perturbed Kohnâ€“Sham Methods. Journal of Physical Chemistry C, 2019, 123, 8336-8346.	1.5	24
13	Thermal properties of the orthorhombic CaSnO3 perovskite under pressure from ab initio quasi-harmonic calculations. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	22
14	Quasiâ€Harmonic Lattice Dynamics of a Prototypical Metalâ€“Organic Framework. Advanced Theory and Simulations, 2019, 2, 1900093.	1.3	21
15	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.	1.9	21
16	Hydrostatic and [001] Uniaxial Pressure on Anatase TiO₂ by Periodic B3LYP-D* Calculations. Journal of Physical Chemistry C, 2013, 117, 7050-7061.	1.5	20
17	Thermoelasticity in organic semiconductors determined with terahertz spectroscopy and quantum quasi-harmonic simulations. Journal of Materials Chemistry C, 2020, 8, 10917-10925.	2.7	20
18	Influence of the synthesis media in the properties of CuO obtained by microwave-assisted hydrothermal method. Journal of Thermal Analysis and Calorimetry, 2011, 106, 519-523.	2.0	19

#	Article	IF	Citations
19	Thermoelasticity of Flexible Organic Crystals from Quasi-harmonic Lattice Dynamics: The Case of Copper(II) Acetylacetonate. Journal of Physical Chemistry Letters, 2020, 11, 8543-8548.	2.1	15
20	A quantum-mechanical investigation of oxygen vacancies and copper doping in the orthorhombic CaSnO₃ perovskite. Physical Chemistry Chemical Physics, 2018, 20, 20970-20980.	1.3	10
21	Elucidating the structure and dynamics of CO ad-layers on MgO surfaces. Physical Chemistry Chemical Physics, 2019, 21, 26279-26283.	1.3	10
22	Anharmonic Coupling of Stretching Vibrations in Ice: A Periodic VSCF and VCI Description. Journal of Chemical Theory and Computation, 2022, 18, 4428-4437.	2.3	10
23	Nitrogen interstitial defects in silicon. A quantum mechanical investigation of the structural, electronic and vibrational properties. Materials Today Communications, 2019, 21, 100616.	0.9	9
24	Estimation of the oxidation temperature of biodiesels from a limited number of chemical parameters. Fuel, 2012, 102, 585-591.	3.4	6
25	The first step of biodiesel autoxidation by differential scanning calorimetry and DFT calculations. Journal of Thermal Analysis and Calorimetry, 2014, 117, 799-806.	2.0	4
26	Structural and Mechanical Properties of Metal-Organic Frameworks Probed with Terahertz Time-Domain Spectroscopy. , 2018, , .		0
27	Ultra Fast Hematite Preparation using a Microwave-Assisted Hydrothermal Method. Current Physical Chemistry, 2013, 3, 477-484.	0.1	0