Iurii Timrov

List of Publications by Year
in descending order

28	6,078	430874 18	454955 30
papers	citations	h-index	g-index

31	31	31	7671
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	HP â€“ A code for the calculation of Hubbard parameters using density-functional perturbation theory. Computer Physics Communications, 2022, 279, 108455.	7.5	35
2	Self-consistent Hubbard parameters from density-functional perturbation theory in the ultrasoft and projector-augmented wave formulations. Physical Review B, 2021, 103, .	3.2	84
3	Extensive Benchmarking of DFT+U Calculations for Predicting Band Gaps. Applied Sciences (Switzerland), 2021, 11, 2395.	2.5	75
4	Virtual Computational Chemistry Teaching Laboratoriesâ€”Hands-On at a Distance. Journal of Chemical Education, 2021, 98, 3163-3171.	2.3	15
5	AbÂInitio Electron-Phonon Interactions in Correlated Electron Systems. Physical Review Letters, 2021, 127, 126404.	7.8	22
6	Coherent energy exchange between carriers and phonons in Peierls-distorted bismuth unveiled by broadband XUV pulses. Physical Review Research, 2021, 3, .	3.6	8
7	Optimizing accuracy and efficacy in data-driven materials discovery for the solar production of hydrogen. Energy and Environmental Science, 2021, 14, 2335-2348.	30.8	23
8	Importance of intersite Hubbard interactions in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î²</mml:mi><mml:mtext>â^'</mml:mtext><mml:msub><mml:mrow><r : A first-principles <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi><mml:r study. Physical Review Materials, 2021, 5, .	2.4	12
9	Electron energy loss spectroscopy of bulk gold with ultrasoft pseudopotentials and the Liouville-Lanczos method. Physical Review B, 2020, 102, .	3.2	8
10	Hubbard-corrected density functional perturbation theory with ultrasoft pseudopotentials. Physical Review B, 2020, 101, .	3.2	43
11	Q<scp>uantum</scp> ESPRESSO toward the exascale. Journal of Chemical Physics, 2020, 152, 154105.	3.0	796
12	Pulay forces in density-functional theory with extended Hubbard functionals: From nonorthogonalized to orthogonalized manifolds. Physical Review B, 2020, 102, .	3.2	22
13	Self-consistent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi><mml:r study of oxygen vacancies in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><m	3.6	50
14	Electronic structure of pristine and Ni-substituted <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>La</mml:mi><mml:mi>Fe</mml:mi><mml:msub><mml:m mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> from near edge x-ray absorption fine structure experiments and first-principles simulations. Physical	3.6	17
15	Self-consistent site-dependent DFT+ <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math> study of stoichiometric and defective <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrMnO</mml:mi><mml:mn>3</mml:mn></mml:msub><m Physical Review B, 2019, 99, .	3.2	39
16	Spin dynamics from time-dependent density functional perturbation theory. European Physical Journal B, 2018, 91, 1.	1.5	17
17	Hubbard parameters from density-functional perturbation theory. Physical Review B, 2018, 98, .	3.2	194
18	Ab initiostudy of electron energy loss spectra of bulk bismuth up to 100 eV. Physical Review B, 2017, 95, .	3.2	10

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19	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
20	Multimodel Approach to the Optical Properties of Molecular Dyes in Solution. Journal of Chemical Theory and Computation, 2016, 12, 4423-4429.	5.3	13
21	turboEELSâ€"A code for the simulation of the electron energy loss and inelastic X-ray scattering spectra using the Liouvilleâ€"Lanczos approach to time-dependent density-functional perturbation theory. Computer Physics Communications, 2015, 196, 460-469.	7.5	41
22	Self-consistent continuum solvation for optical absorption of complex molecular systems in solution. Journal of Chemical Physics, 2015, 142, 034111.	3.0	17
23	Accurate and Inexpensive Prediction of the Color Optical Properties of Anthocyanins in Solution. Journal of Physical Chemistry A, 2015, 119, 3816-3822.	2.5	36
24	FIRST-PRINCIPLES CALCULATIONS OF ELECTRON-PHONON SCATTERING. Annual Review of Heat Transfer, 2014, 17, 333-383.	1.0	7
25	Direct observation of electron thermalization and electron-phonon coupling in photoexcited bismuth. Physical Review B, 2013, 88, .	3.2	48
26	Electron energy loss and inelastic x-ray scattering cross sections from time-dependent density-functional perturbation theory. Physical Review B, 2013, 88, .	3.2	29
27	Thermalization of photoexcited carriers in bismuth investigated by time-resolved terahertz spectroscopy andab initiocalculations. Physical Review B, 2012, 85, .	3.2	34
28	Coherent Phonon Coupling to Individual Bloch States in Photoexcited Bismuth. Physical Review Letters, 2012, 108, 256808.	7.8	70