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	Advanced capabilities for materials modelling with Quantum ESPRESSO. Journal of Physics Condensed Matter, 2017, 29, 465901.	1.8	4,303
2	Q<scp>uantum</scp> ESPRESSO toward the exascale. Journal of Chemical Physics, 2020, 152, 154105.	3.0	796
3	Hubbard parameters from density-functional perturbation theory. Physical Review B, 2018, 98, .	3.2	194
4	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
5	Extensive Benchmarking of DFT+U Calculations for Predicting Band Gaps. Applied Sciences (Switzerland), 2021, 11, 2395.	2.5	75
6	Coherent Phonon Coupling to Individual Bloch States in Photoexcited Bismuth. Physical Review Letters, 2012, 108, 256808.	7.8	70
7	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> 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> Physical Review Research, 2020, 2, .	3.6	50
8	Direct observation of electron thermalization and electron-phonon coupling in photoexcited bismuth. Physical Review B, 2013, 88, .	3.2	48
9	Hubbard-corrected density functional perturbation theory with ultrasoft pseudopotentials. Physical Review B, 2020, 101, .	3.2	43
10	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
11	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> Physical Review B, 2018, 98, .	3.2	39
12	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
13	HP â€“ A code for the calculation of Hubbard parameters using density-functional perturbation theory. Computer Physics Communications, 2022, 279, 108455.	7.5	35
14	Thermalization of photoexcited carriers in bismuth investigated by time-resolved terahertz spectroscopy andab initiocalculations. Physical Review B, 2012, 85, .	3.2	34
15	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
16	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
17	AbÂInitio Electron-Phonon Interactions in Correlated Electron Systems. Physical Review Letters, 2021, 127, 126404.	7.8	22
18	Pulay forces in density-functional theory with extended Hubbard functionals: From nonorthogonalized to orthogonalized manifolds. Physical Review B, 2020, 102, .	3.2	22

#	Article	IF	Citations
19	Self-consistent continuum solvation for optical absorption of complex molecular systems in solution. Journal of Chemical Physics, 2015, 142, 034111.	3.0	17
20	Spin dynamics from time-dependent density functional perturbation theory. European Physical Journal B, 2018, 91, 1.	1.5	17
21	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:mi 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 Review Research, 2020, 2, .	3.6	17
22	Virtual Computational Chemistry Teaching Laboratoriesâ€”Hands-On at a Distance. Journal of Chemical Education, 2021, 98, 3163-3171.	2.3	15
23	Multimodel Approach to the Optical Properties of Molecular Dyes in Solution. Journal of Chemical Theory and Computation, 2016, 12, 4423-4429.	5.3	13
24	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
25	Ab initiostudy of electron energy loss spectra of bulk bismuth up to 100 eV. Physical Review B, 2017, 95, .	3.2	10
26	Electron energy loss spectroscopy of bulk gold with ultrasoft pseudopotentials and the Liouville-Lanczos method. Physical Review B, 2020, 102, .	3.2	8
27	Coherent energy exchange between carriers and phonons in Peierls-distorted bismuth unveiled by broadband XUV pulses. Physical Review Research, 2021, 3, .	3.6	8
28	FIRST-PRINCIPLES CALCULATIONS OF ELECTRON-PHONON SCATTERING. Annual Review of Heat Transfer, 2014, 17, 333-383.	1.0	7