Andris Gulans

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1102806/publications.pdf

Version: 2024-02-01

30 papers	3,200 citations	516710 16 h-index	477307 29 g-index
31 all docs	31 docs citations	31 times ranked	5598 citing authors

#	Article	IF	Citations
1	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
2	van der Waals Bonding in Layered Compounds from Advanced Density-Functional First-Principles Calculations. Physical Review Letters, 2012, 108, 235502.	7.8	851
3	exciting: a full-potential all-electron package implementing density-functional theory and many-body perturbation theory. Journal of Physics Condensed Matter, 2014, 26, 363202.	1.8	241
4	Electronic structure of boron nitride sheets doped with carbon from first-principles calculations. Physical Review B, 2013, 87, .	3.2	162
5	Linear-scaling self-consistent implementation of the van der Waals density functional. Physical Review B, 2009, 79, .	3.2	151
6	Are we van der Waals ready?. Journal of Physics Condensed Matter, 2012, 24, 424218.	1.8	129
7	Role of van der Waals interaction in forming molecule-metal junctions: flat organic molecules on the Au(111) surface. Physical Chemistry Chemical Physics, 2010, 12, 4759.	2.8	109
8	Cathodoluminescence of Ge+, Si+, and O+ implanted SiO2 layers and the role of mobile oxygen in defect transformations. Journal of Non-Crystalline Solids, 2002, 303, 218-231.	3.1	86
9	Accurate all-electron<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>G</mml:mi><mml:mn>0</mml:mn></mml:msub></mml:mrow></mml:math>W<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>0</mml:mi></mml:msub></mml:mrow></mml:math> energies employing the full-potential augmented plane-wave method. Physical Review B, 2016, 94, .	3.2	77
10	Bound and free self-interstitial defects in graphite and bilayer graphene: A computational study. Physical Review B, 2011, 84, .	3.2	32
11	Lennardâ€Jones parameters for small diameter carbon nanotubes and water for molecular mechanics simulations from van der Waals density functional calculations. Journal of Computational Chemistry, 2012, 33, 652-658.	3.3	31
12	Ab initio calculation of wurtzite-type GaN nanowires. Physica Status Solidi C: Current Topics in Solid State Physics, 2007, 4, 1197-1200.	0.8	25
13	Towards numerically accurate many-body perturbation theory: Short-range correlation effects. Journal of Chemical Physics, 2014, 141, 164127.	3.0	24
14	Microhartree precision in density functional theory calculations. Physical Review B, 2018, 97, .	3.2	23
15	Twoâ€Dimensional Nanostructured Growth of Nanoclusters and Molecules on Insulating Surfaces. Advanced Materials, 2012, 24, 3228-3232.	21.0	22
16	Graphene-modulated photo-absorption in adsorbed azobenzene monolayers. Physical Chemistry Chemical Physics, 2017, 19, 6196-6205.	2.8	21
17	Adsorption structures of phenol on theSi(001)â^'(2Ã—1)surface calculated using density functional theory. Physical Review B, 2010, 81, .	3.2	15
18	Acetylene adsorption on silicon (100)-(4Ã—2) revisited. Surface Science, 2011, 605, 1341-1346.	1.9	14

#	Article	IF	Citations
19	Electronic and Optical Excitations at the Pyridine/ZnO(101Â¯0) Hybrid Interface. Advanced Theory and Simulations, 2019, 2, 1800108.	2.8	13
20	Ab initio calculations of charged point defects in GaN. Physica Status Solidi C: Current Topics in Solid State Physics, 2005, 2, 507-510.	0.8	12
21	Critical Importance of van der Waals Stabilization in Strongly Chemically Bonded Surfaces: Cu(110):O. Journal of Chemical Theory and Computation, 2013, 9, 5578-5584.	5.3	10
22	The LDA-1/2 Method Applied to Atoms and Molecules. Journal of Chemical Theory and Computation, 2018, 14, 4678-4686.	5.3	8
23	The LDA-1/2 method implemented in the excitingÂcode. Computer Physics Communications, 2017, 220, 263-268.	7.5	7
24	Maximally localized Wannier functions within the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>(</mml:mo><mml:mi) Tj ETQq0 0 0 rgBT /Overlock 10 Tf method. Physical Review B, 2020, 101, .	3.2	6
25	Numerical quality control for DFT-based materials databases. Npj Computational Materials, 2022, 8, .	8.7	6
26	Luminescence and electron transport properties of GaN and AlN layers. Radiation Measurements, 2001, 33, 709-713.	1.4	5
27	Robust mixing in self-consistent linearized augmented planewave calculations. Electronic Structure, 2020, 2, 037001.	2.8	5
28	Surfaces: Two-Dimensional Nanostructured Growth of Nanoclusters and Molecules on Insulating Surfaces (Adv. Mater. 24/2012). Advanced Materials, 2012, 24, 3146-3146.	21.0	1
29	Work-function modification of PEG(thiol) adsorbed on the Au(111) surface: A first-principles study. Physical Review Materials, 2020, 4, .	2.4	1
30	LCAO calculation of neutral defects in GaN. Physica Status Solidi C: Current Topics in Solid State Physics, 2005, 2, 2525-2528.	0.8	0