Per Hyldgaard

List of Publications by Year
in descending order

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		101543	51608
104	7,521	36	86
papers	citations	h-index	g-index

106	106	106	7353
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Hard and soft materials: putting consistent van der Waals density functionals to work. Electronic Structure, 2022, 4, 014001.	2.8	4
2	An assessment of density functionals for predicting CO2 adsorption in diamine-functionalized metalâ€“organic frameworks. Journal of Chemical Physics, 2022, 156, 154113.	3.0	7
3	vdW-DF-ahcx: a range-separated van der Waals density functional hybrid. Journal of Physics Condensed Matter, 2021, 34, .	1.8	7
4	Unraveling the Ground-State Structure of BaZrO₃ by Neutron Scattering Experiments and First-Principles Calculations. Chemistry of Materials, 2020, 32, 2824-2835.	6.7	41
5	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BaZrO</mml:mi><mml:mn>3</mml:mn></mml:msub></m stability under pressure: The role of nonlocal exchange and correlation. Physical Review B, 2020, 101, .	3.2	12
6	Screening nature of the van der Waals density functional method: a review and analysis of the many-body physics foundation. Journal of Physics Condensed Matter, 2020, 32, 393001.	1.8	28
7	First-principles study of the binding energy between nanostructures and its scaling with system size. Physical Review B, 2018, 97, .	3.2	13
8	Signatures of van der Waals binding: A coupling-constant scaling analysis. Physical Review B, 2018, 97, .	3.2	17
9	Understanding noninvasive charge transfer doping of graphene: a comparative study. Journal of Materials Science: Materials in Electronics, 2018, 29, 5239-5252.	2.2	14
10	Extent of Fock-exchange mixing for a hybrid van der Waals density functional?. Journal of Chemical Physics, 2018, 148, 194115.	3.0	17
11	Ab initioinvestigation of monoclinic phase stability and martensitic transformation in crystalline polyethylene. Physical Review Materials, 2018, 2, .	2.4	14
12	Ab initio and classical atomistic modelling of structure and defects inÂcrystalline orthorhombic polyethylene: Twin boundaries, slip interfaces, and nature of barriers. Polymer, 2017, 121, 234-246.	3.8	19
13	libvdwxc: a library for exchangeâ€“correlation functionals in the vdW-DF family. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 065004.	2.0	28
14	Assessment of two hybrid van der Waals density functionals for covalent and non-covalent binding of molecules. Journal of Chemical Physics, 2017, 146, 234106.	3.0	33
15	Finite-temperature properties of nonmagnetic transition metals: Comparison of the performance of constraint-based semilocal and nonlocal functionals. Physical Review B, 2017, 95, .	3.2	35
16	The vdW-DF Family of Nonlocal Exchange-Correlation Functionals. , 2017, , 241-274.		8
17	Optimization of Norbornadiene Compounds for Solar Thermal Storage by Firstâ€Principles Calculations. ChemSusChem, 2016, 9, 1786-1794.	6.8	38
18	A Mechanism for Highly Efficient Electrochemical Bubbling Delamination of CVDâ€Grown Graphene from Metal Substrates. Advanced Materials Interfaces, 2016, 3, 1500492.	3.7	33

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19	Optimization of Norbornadiene Compounds for Solar Thermal Storage by First-Principles Calculations. ChemSusChem, 2016, 9, 1745-1745.	6.8	2
20	Comparative Ab-Initio Study of Substituted Norbornadiene-Quadricyclane Compounds for Solar Thermal Storage. Journal of Physical Chemistry C, 2016, 120, 3635-3645.	3.1	71
21	Structural and excited-state properties of oligoacene crystals from first principles. Physical Review B, 2016, 93, .	3.2	89
22	Spin Signature of Nonlocal Correlation Binding in Metal-Organic Frameworks. Physical Review Letters, 2015, 115, 136402.	7.8	272
23	van der Waals forces in density functional theory: a review of the vdW-DF method. Reports on Progress in Physics, 2015, 78, 066501.	20.1	615
24	Microscopic Origin of Thermal Conductivity Reduction in Disordered van der Waals Solids. Chemistry of Materials, 2015, 27, 5511-5518.	6.7	33
25	van der Waals density functionals built upon the electron-gas tradition: Facing the challenge of competing interactions. Journal of Chemical Physics, 2014, 140, 18A539.	3.0	100
26	Exchange functional that tests the robustness of the plasmon description of the van der Waals density functional. Physical Review B, 2014, 89, .	3.2	414
27	Interpretation of van der Waals density functionals. Physical Review B, 2014, 90, .	3.2	63
28	Analysis of van der Waals density functional components: Binding and corrugation of benzene and C<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>60</mml:mn></mml:msub></mml:math>on boron nitride and graphene. Physical Review B, 2013, 87, .	3.2	95
29	Harris-type van der Waals density functional scheme. Physical Review B, 2013, 88, .	3.2	8
30	Response of the Shockley surface state to an external electrical field: A density-functional theory study of Cu(111). Physical Review B, 2012, 85, .	3.2	19
31	Nonequilibrium thermodynamics of interacting tunneling transport: variational grand potential, density functional formulation and nature of steady-state forces. Journal of Physics Condensed Matter, 2012, 24, 424219.	1.8	14
32	Design and Fabrication of AlN/GaN Heterostructures for Intersubband Technology. Japanese Journal of Applied Physics, 2012, 51, 01AG07.	1.5	1
33	Van der Waals interactions in advanced materials, in memory of David C Langreth. Journal of Physics Condensed Matter, 2012, 24, 420201.	1.8	2
34	Physisorption of nucleobases on graphene: a comparative van der Waals study. Journal of Physics Condensed Matter, 2012, 24, 424210.	1.8	83
35	Benchmarking van der Waals density functionals with experimental data: potential-energy curves for H₂molecules on Cu(111), (100) and (110) surfaces. Journal of Physics Condensed Matter, 2012, 24, 424213.	1.8	35
36	Design and Fabrication of AlN/GaN Heterostructures for Intersubband Technology. Japanese Journal of Applied Physics, 2012, 51, 01AG07.	1.5	2

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37	Do Two-Dimensional â€œNoble Gas Atomsâ€•Produce Molecular Honeycombs at a Metal Surface?. Nano Letters, 2011, 11, 2944-2948.	9.1	33
38	Polarization-balanced design of heterostructures: Application to AlN/GaN double-barrier structures. Physical Review B, 2011, 84, .	3.2	15
39	Waveguides for nitride based quantum cascade lasers. Physica Status Solidi C: Current Topics in Solid State Physics, 2011, 8, 2357-2359.	0.8	10
40	Van der Waals density functional calculations of binding in molecular crystals. Computer Physics Communications, 2011, 182, 1800-1804.	7.5	44
41	Computational scheme for ab-initio predictions of chemical compositions interfaces realized by deposition growth. Computer Physics Communications, 2011, 182, 1814-1818.	7.5	1
42	Evaluation of a density functional with account of van der Waals forces using experimental data of H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>physisorption on Cu(111). Physical Review B, 2011, 84, .	3.2	46
43	Graphene nanogap for gate-tunable quantum-coherent single-molecule electronics. Physical Review B, 2011, 84, .	3.2	25
44	Stacking and band structure of van der Waals bonded graphane multilayers. Physical Review B, 2011, 83, .	3.2	44
45	Effective elastic properties of a van der Waals molecular monolayer at a metal surface. Physical Review B, 2010, 82, .	3.2	18
46	Temperature stability of intersubband transitions in AlN/GaN quantum wells. Applied Physics Letters, 2010, 97, 043507.	3.3	16
47	Structure and binding in crystals of cagelike molecules: Hexamine and platonic hydrocarbons. Journal of Chemical Physics, 2010, 132, 134705.	3.0	34
48	Ab initiothermodynamics of deposition growth: Surface terminations of TiC(111) and TiN(111) grown by chemical vapor deposition. Physical Review B, 2010, 82, .	3.2	8
49	Publisher's Note: Effective elastic properties of a van der Waals molecular monolayer at a metal surface [Phys. Rev. B82, 201410 (2010)]. Physical Review B, 2010, 82, .	3.2	0
50	Ab initiostructure modelling of complex thin-film oxides: thermodynamical stability of TiC/thin-film alumina. Journal of Physics Condensed Matter, 2010, 22, 015004.	1.8	4
51	Understanding adhesion at as-deposited interfaces fromab initiothermodynamics of deposition growth: thin-film alumina on titanium carbide. Journal of Physics Condensed Matter, 2010, 22, 472001.	1.8	3
52	Binding of polycyclic aromatic hydrocarbons and graphene dimers in density functional theory. New Journal of Physics, 2010, 12, 013017.	2.9	55
53	Rings sliding on a honeycomb network: Adsorption contours, interactions, and assembly of benzene on Cu(111). Physical Review B, 2009, 80, .	3.2	73
54	A density functional for sparse matter. Journal of Physics Condensed Matter, 2009, 21, 084203.	1.8	363

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55	Band bending and quasiâ€2DEG in the metallized Î²â€SiC(001) surface. Physica Status Solidi - Rapid Research Letters, 2008, 2, 218-220.	2.4	9
56	Coarse-grained model for growth of Î±- and ƙ-Al2O3on TiC and TiN(111): thin alumina films from density-functional calculations. Journal of Physics: Conference Series, 2008, 100, 082010.	0.4	2
57	Density-functional theory of nonequilibrium tunneling. Physical Review B, 2008, 78, .	3.2	9
58	Nature and strength of bonding in a crystal of semiconducting nanotubes: van der Waals density functional calculations and analytical results. Physical Review B, 2008, 77, .	3.2	53
59	Adsorption of methylamine onÎ±â^'Al2O3(0001)andÎ±â^'Cr2O3(0001): Density functional theory. Physical Review B, 2007, 75, .	3.2	34
60	Potassium intercalation in graphite: A van der Waals density-functional study. Physical Review B, 2007, 76, .	3.2	155
61	Van der Waals density functional: Self-consistent potential and the nature of the van der Waals bond. Physical Review B, 2007, 76, .	3.2	1,058
62	TEM and DFT investigation of CVD TiN/Îºâ€“Al2O3 multilayer coatings. Surface and Coatings Technology, 2007, 202, 522-531.	4.8	16
63	Phonon Knudsen flow in nanostructured semiconductor systems. Journal of Applied Physics, 2006, 99, 054303.	2.5	22
64	Thermal transport in SiC nanostructures. Materials Science and Engineering C, 2005, 25, 635-640.	7.3	9
65	Interactions mediated by surface states: from pairs and trios to adchains and ordered overlayers. Journal of Crystal Growth, 2005, 275, e1637-e1642.	1.5	12
66	Van der Waals density functional theory with applications. International Journal of Quantum Chemistry, 2005, 101, 599-610.	2.0	304
67	One-dimensional electron systems for anchoring growth of carbon nanostructures. Computational Materials Science, 2005, 33, 356-361.	3.0	1
68	First stages of the oxidation of the Si-rich 3Câ€“SiC(001) surface. Computational Materials Science, 2005, 33, 13-19.	3.0	9
69	Van der Waals interaction of parallel polymers and nanotubes. Computational Materials Science, 2005, 33, 192-199.	3.0	22
70	Quantum Confinement in Monatomic Cu Chains on Cu(111). Physical Review Letters, 2004, 92, 056803.	7.8	186
71	Resonant thermal transport in semiconductor barrier structures. Physical Review B, 2004, 69, .	3.2	10
72	First-Principles Study of O Adsorption at SiC Surface. Materials Science Forum, 2004, 457-460, 1293-1296.	0.3	3

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73	Quantum wire behavior in a one-component metallic system: monatomic Cu chains on Cu(111). Physica E: Low-Dimensional Systems and Nanostructures, 2004, 24, 111-114.	2.7	3
74	Van der Waals Density Functional for Layered Structures. Physical Review Letters, 2003, 91, 126402.	7.8	623
75	Van der Waals interactions of parallel and concentric nanotubes. Materials Science and Engineering C, 2003, 23, 721-725.	7.3	33
76	Hard numbers on soft matter. Surface Science, 2003, 532-535, 606-610.	1.9	76
77	Hard-materials-surface prediction of one-dimensional electron gas. Surface Science, 2003, 532-535, 594-599.	1.9	0
78	Surface-state mediated three-adsorbate interaction: electronic nature and nanoscale consequences. Surface Science, 2003, 532-535, 600-605.	1.9	15
79	The van der Waals interactions of concentric nanotubes. Surface Science, 2003, 532-535, 880-885.	1.9	14
80	Surface-state mediated three-adsorbate interaction: exact and numerical results and simple asymptotic expression. Applied Surface Science, 2003, 212-213, 856-860.	6.1	6
81	Control of molecular excitations in nanotube-heterostructure transistors. Materials Science and Engineering C, 2003, 23, 243-246.	7.3	8
82	Self-Organized One-Dimensional Electron Systems on a Low-Symmetry Oxide Surface. Physical Review Letters, 2003, 90, 236803.	7.8	5
83	Site Determination and Thermally Assisted Tunneling in Homogenous Nucleation. Physical Review Letters, 2003, 91, 206102.	7.8	105
84	Surface-stateâ€“mediated three-adsorbate interaction. Europhysics Letters, 2002, 59, 265-271.	2.0	37
85	Bridging between micro- and macroscales of materials by mesoscopic models. Computational Materials Science, 2002, 24, 1-13.	3.0	4
86	Hydrogen dynamics in magnesium and graphite. Computational Materials Science, 2002, 24, 273-277.	3.0	58
87	Transport in robust fullerene-tube heterostructure transistor. Materials Science and Engineering C, 2002, 19, 445-448.	7.3	4
88	Density-functional bridge between surfaces and interfaces. Surface Science, 2001, 493, 253-270.	1.9	31
89	Low-temperature control of nanoscale molecular dynamics. Low Temperature Physics, 2001, 27, 585-589.	0.6	6
90	Density-functional calculation of van der Waals forces for free-electron-like surfaces. Physical Review B, 2001, 64, .	3.2	49

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91	Robust nanosized transistor effect in fullerene-tube heterostructure. Solid State Communications, 2000, 116, 569-573.	1.9	19
92	Substrate Mediated Long-Range Oscillatory Interaction between Adatoms: Cu/Cu(111). Physical Review Letters, 2000, 85, 2981-2984.	7.8	363
93	Nature, Strength, and Consequences of Indirect Adsorbate Interactions on Metals. Physical Review Letters, 2000, 85, 1910-1913.	7.8	175
94	Long-ranged adsorbate-adsorbate interactions mediated by a surface-state band. Journal of Physics Condensed Matter, 2000, 12, L13-L19.	1.8	152
95	Al Dimer Dynamics on Al(111). Physical Review Letters, 1998, 81, 172-175.	7.8	52
96	Phonon superlattice transport. Physical Review B, 1997, 56, 10754-10757.	3.2	203
97	Electron-electron scattering in far-infrared quantum cascade lasers. Physical Review B, 1996, 53, 6889-6892.	3.2	49
98	Resonant Tunneling with an Electron-Phonon Interaction. Annals of Physics, 1994, 236, 1-42.	2.8	62
99	Current and rate equation for resonant tunneling. Physical Review B, 1993, 47, 4603-4618.	3.2	62
100	Zero-frequency current noise for the double-tunnel-junction Coulomb blockade. Physical Review B, 1993, 47, 1967-1979.	3.2	155
101	Noise as a diagnostic of tunneling mechanisms. Physica Scripta, 1992, T42, 115-121.	2.5	17
102	Classical theory for shot noise in resonant tunneling. Physical Review B, 1992, 46, 9620-9633.	3.2	117
103	Elastic and inelastic resonant tunnelling in narrow-band systems: application to transport in minibands of semiconductor superlattices. Journal of Physics Condensed Matter, 1990, 2, 8725-8729.	1.8	12
104	Scaling relations at the critical line and the period-doubling route for the sine map and the driven damped pendulum. Physical Review A, 1986, 34, 2220-2233.	2.5	14