Per Hyldgaard

List of Publications by Year in Descending Order

103 papers	6,517 citations	35 h-index	80 g-index
106 ext. papers	7,090 ext. citations	3.8 avg, IF	5.81 L-index

#	Paper	IF	Citations
103	Hard and soft materials: putting consistent van der Waals density functionals to work. *Electronic Structure*, **2022**, 4, 014001	2.6	1
102	An assessment of density functionals for predicting CO adsorption in diamine-functionalized metal-organic frameworks.. *Journal of Chemical Physics*, **2022**, 156, 154113	3.9	0
101	vdW-DF-ahcx: a range-separated van der Waals density functional hybrid. *Journal of Physics Condensed Matter*, **2021**, 34,	1.8	2
100	Unraveling the Ground-State Structure of BaZrO3 by Neutron Scattering Experiments and First-Principles Calculations. *Chemistry of Materials*, **2020**, 32, 2824-2835	9.6	17
99	BaZrO3 stability under pressure: The role of nonlocal exchange and correlation. *Physical Review B*, **2020**, 101,	3.3	4
98	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	19
97	First-principles study of the binding energy between nanostructures and its scaling with system size. *Physical Review B*, **2018**, 97,	3.3	12
96	Signatures of van der Waals binding: A coupling-constant scaling analysis. *Physical Review B*, **2018**, 97,	3.3	12
95	Understanding noninvasive charge transfer doping of graphene: a comparative study. *Journal of Materials Science: Materials in Electronics*, **2018**, 29, 5239-5252	2.1	8
94	Ab initio investigation of monoclinic phase stability and martensitic transformation in crystalline polyethylene. *Physical Review Materials*, **2018**, 2,	3.2	8
93	Extent of Fock-exchange mixing for a hybrid van der Waals density functional?. *Journal of Chemical Physics*, **2018**, 148, 194115	3.9	11
92	Ab initio and classical atomistic modelling of structure and defects in crystalline orthorhombic polyethylene: Twin boundaries, slip interfaces, and nature of barriers. *Polymer*, **2017**, 121, 234-246	3.9	13
91	libvdwxc: a library for exchange correlation functionals in the vdW-DF family. *Modelling and Simulation in Materials Science and Engineering*, **2017**, 25, 065004	2	21
90	The vdW-DF Family of Nonlocal Exchange-Correlation Functionals **2017**, 241-274		5
89	Assessment of two hybrid van der Waals density functionals for covalent and non-covalent binding of molecules. *Journal of Chemical Physics*, **2017**, 146, 234106	3.9	28
88	Finite-temperature properties of nonmagnetic transition metals: Comparison of the performance of constraint-based semilocal and nonlocal functionals. *Physical Review B*, **2017**, 95,	3.3	32
87	Structural and excited-state properties of oligoacene crystals from first principles. *Physical Review B*, **2016**, 93,	3.3	73

86	Optimization of Norbornadiene Compounds for Solar Thermal Storage by First-Principles Calculations. *ChemSusChem*, **2016**, 9, 1786-94	8.3	27
85	A Mechanism for Highly Efficient Electrochemical Bubbling Delamination of CVD-Grown Graphene from Metal Substrates. *Advanced Materials Interfaces*, **2016**, 3, 1500492	4.6	28
84	Optimization of Norbornadiene Compounds for Solar Thermal Storage by First-Principles Calculations. *ChemSusChem*, **2016**, 9, 1745-1745	8.3	1
83	Comparative Ab-Initio Study of Substituted Norbornadiene-Quadricyclane Compounds for Solar Thermal Storage. *Journal of Physical Chemistry C*, **2016**, 120, 3635-3645	3.8	54
82	van der Waals forces in density functional theory: a review of the vdW-DF method. *Reports on Progress in Physics*, **2015**, 78, 066501	14.4	477
81	Microscopic Origin of Thermal Conductivity Reduction in Disordered van der Waals Solids. *Chemistry of Materials*, **2015**, 27, 5511-5518	9.6	27
80	Spin Signature of Nonlocal Correlation Binding in Metal-Organic Frameworks. *Physical Review Letters*, **2015**, 115, 136402	7.4	189
79	Interpretation of van der Waals density functionals. *Physical Review B*, **2014**, 90,	3.3	57
78	van der Waals density functionals built upon the electron-gas tradition: facing the challenge of competing interactions. *Journal of Chemical Physics*, **2014**, 140, 18A539	3.9	86
77	Exchange functional that tests the robustness of the plasmon description of the van der Waals density functional. *Physical Review B*, **2014**, 89,	3.3	319
76	Analysis of van der Waals density functional components: Binding and corrugation of benzene and C60 on boron nitride and graphene. *Physical Review B*, **2013**, 87,	3.3	87
75	Harris-type van der Waals density functional scheme. *Physical Review B*, **2013**, 88,	3.3	6
74	Physisorption of nucleobases on graphene: a comparative van der Waals study. *Journal of Physics Condensed Matter*, **2012**, 24, 424210	1.8	72
73	Benchmarking van der Waals density functionals with experimental data: potential-energy curves for H2 molecules on Cu(111), (100) and (110) surfaces. *Journal of Physics Condensed Matter*, **2012**, 24, 424213	1.8	33
72	Response of the Shockley surface state to an external electrical field: A density-functional theory study of Cu(111). *Physical Review B*, **2012**, 85,	3.3	18
71	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	10
70	Design and Fabrication of AlN/GaN Heterostructures for Intersubband Technology. *Japanese Journal of Applied Physics*, **2012**, 51, 01AG07	1.4	1
69	Design and Fabrication of AlN/GaN Heterostructures for Intersubband Technology. *Japanese Journal of Applied Physics*, **2012**, 51, 01AG07	1.4	2

68	Polarization-balanced design of heterostructures: Application to AlN/GaN double-barrier structures. *Physical Review B*, **2011**, 84,	3.3	14
67	Waveguides for nitride based quantum cascade lasers. *Physica Status Solidi C: Current Topics in Solid State Physics*, **2011**, 8, 2357-2359		10
66	Do two-dimensional "noble gas atoms" produce molecular honeycombs at a metal surface?. *Nano Letters*, **2011**, 11, 2944-8	11.5	30
65	Van der Waals density functional calculations of binding in molecular crystals. *Computer Physics Communications*, **2011**, 182, 1800-1804	4.2	42
64	Computational scheme for ab-initio predictions of chemical compositions interfaces realized by deposition growth. *Computer Physics Communications*, **2011**, 182, 1814-1818	4.2	1
63	Evaluation of a density functional with account of van der Waals forces using experimental data of H2 physisorption on Cu(111). *Physical Review B*, **2011**, 84,	3.3	44
62	Graphene nanogap for gate-tunable quantum-coherent single-molecule electronics. *Physical Review B*, **2011**, 84,	3.3	24
61	Stacking and band structure of van der Waals bonded graphane multilayers. *Physical Review B*, **2011**, 83,	3.3	43
60	Effective elastic properties of a van der Waals molecular monolayer at a metal surface. *Physical Review B*, **2010**, 82,	3.3	18
59	Temperature stability of intersubband transitions in AlN/GaN quantum wells. *Applied Physics Letters*, **2010**, 97, 043507	3.4	16
58	Structure and binding in crystals of cagelike molecules: hexamine and platonic hydrocarbons. *Journal of Chemical Physics*, **2010**, 132, 134705	3.9	33
57	Ab initio thermodynamics of deposition growth: Surface terminations of TiC(111) and TiN(111) grown by chemical vapor deposition. *Physical Review B*, **2010**, 82,	3.3	8
56	Ab□initio structure modelling of complex thin-film oxides: thermodynamical stability of TiC/thin-film alumina. *Journal of Physics Condensed Matter*, **2010**, 22, 015004	1.8	4
55	Understanding adhesion at as-deposited interfaces from ab initio thermodynamics of deposition growth: thin-film alumina on titanium carbide. *Journal of Physics Condensed Matter*, **2010**, 22, 472001	1.8	3
54	Binding of polycyclic aromatic hydrocarbons and graphene dimers in density functional theory. *New Journal of Physics*, **2010**, 12, 013017	2.9	51
53	Rings sliding on a honeycomb network: Adsorption contours, interactions, and assembly of benzene on Cu(111). *Physical Review B*, **2009**, 80,	3.3	73
52	A density functional for sparse matter. *Journal of Physics Condensed Matter*, **2009**, 21, 084203	1.8	313
51	Coarse-grained model for growth of □and k-Al2O3on TiC and TiN(111): thin alumina films from density-functional calculations. *Journal of Physics: Conference Series*, **2008**, 100, 082010	0.3	2

50	Density-functional theory of nonequilibrium tunneling. *Physical Review B*, **2008**, 78,	3.3	8
49	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,	3.3	50
48	Band bending and quasi-2DEG in the metallized SiC(001) surface. *Physica Status Solidi - Rapid Research Letters*, **2008**, 2, 218-220	2.5	9
47	Van der Waals density functional: Self-consistent potential and the nature of the van der Waals bond. *Physical Review B*, **2007**, 76,	3.3	909
46	TEM and DFT investigation of CVD TiN/Al2O3 multilayer coatings. *Surface and Coatings Technology*, **2007**, 202, 522-531	4.4	14
45	Adsorption of methylamine on Al2O3(0001) and Cr2O3(0001): Density functional theory. *Physical Review B*, **2007**, 75,	3.3	33
44	Potassium intercalation in graphite: A van der Waals density-functional study. *Physical Review B*, **2007**, 76,	3.3	142
43	Phonon Knudsen flow in nanostructured semiconductor systems. *Journal of Applied Physics*, **2006**, 99, 054303	2.5	18
42	One-dimensional electron systems for anchoring growth of carbon nanostructures. *Computational Materials Science*, **2005**, 33, 356-361	3.2	1
41	First stages of the oxidation of the Si-rich 3C SiC(0 0 1) surface. *Computational Materials Science*, **2005**, 33, 13-19	3.2	9
40	Van der Waals interaction of parallel polymers and nanotubes. *Computational Materials Science*, **2005**, 33, 192-199	3.2	21
39	Thermal transport in SiC nanostructures. *Materials Science and Engineering C*, **2005**, 25, 635-640	8.3	7
38	Interactions mediated by surface states: from pairs and trios to adchains and ordered overlayers. *Journal of Crystal Growth*, **2005**, 275, e1637-e1642	1.6	12
37	Van der Waals density functional theory with applications. *International Journal of Quantum Chemistry*, **2005**, 101, 599-610	2.1	292
36	Quantum confinement in monatomic Cu chains on Cu(111). *Physical Review Letters*, **2004**, 92, 056803	7.4	148
35	Resonant thermal transport in semiconductor barrier structures. *Physical Review B*, **2004**, 69,	3.3	10
34	First-Principles Study of O Adsorption at SiC Surface. *Materials Science Forum*, **2004**, 457-460, 1293-1296	0.4	2
33	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	3	3

32	Van der Waals density functional for layered structures. *Physical Review Letters*, **2003**, 91, 126402	7.4	567
31	Van der Waals interactions of parallel and concentric nanotubes. *Materials Science and Engineering C*, **2003**, 23, 721-725	8.3	28
30	Hard numbers on soft matter. *Surface Science*, **2003**, 532-535, 606-610	1.8	71
29	Hard-materials-surface prediction of one-dimensional electron gas. *Surface Science*, **2003**, 532-535, 594-598	1.8	
28	Surface-state mediated three-adsorbate interaction: electronic nature and nanoscale consequences. *Surface Science*, **2003**, 532-535, 600-605	1.8	14
27	The van der Waals interactions of concentric nanotubes. *Surface Science*, **2003**, 532-535, 880-885	1.8	14
26	Surface-state mediated three-adsorbate interaction: exact and numerical results and simple asymptotic expression. *Applied Surface Science*, **2003**, 212-213, 856-860	6.7	6
25	Control of molecular excitations in nanotube-heterostructure transistors. *Materials Science and Engineering C*, **2003**, 23, 243-246	8.3	8
24	Self-organized one-dimensional electron systems on a low-symmetry oxide surface. *Physical Review Letters*, **2003**, 90, 236803	7.4	5
23	Site determination and thermally assisted tunneling in homogenous nucleation. *Physical Review Letters*, **2003**, 91, 206102	7.4	100
22	Transport in robust fullerene-tube heterostructure transistor. *Materials Science and Engineering C*, **2002**, 19, 445-448	8.3	3
21	Surface-state mediated three-adsorbate interaction. *Europhysics Letters*, **2002**, 59, 265-271	1.6	34
20	Bridging between micro- and macroscales of materials by mesoscopic models. *Computational Materials Science*, **2002**, 24, 1-13	3.2	4
19	Hydrogen dynamics in magnesium and graphite. *Computational Materials Science*, **2002**, 24, 273-277	3.2	52
18	Low-temperature control of nanoscale molecular dynamics. *Low Temperature Physics*, **2001**, 27, 585-589	0.7	6
17	Density-functional calculation of van der Waals forces for free-electron-like surfaces. *Physical Review B*, **2001**, 64,	3.3	48
16	Density-functional bridge between surfaces and interfaces. *Surface Science*, **2001**, 493, 253-270	1.8	29
15	Robust nanosized transistor effect in fullerene-tube heterostructure. *Solid State Communications*, **2000**, 116, 569-573	1.6	17

14	Substrate mediated long-range oscillatory interaction between adatoms: Cu /Cu(111). *Physical Review Letters*, **2000**, 85, 2981-4	7.4	337
13	Nature, strength, and consequences of indirect adsorbate interactions on metals. *Physical Review Letters*, **2000**, 85, 1910-3	7.4	167
12	Long-ranged adsorbate-adsorbate interactions mediated by a surface-state band. *Journal of Physics Condensed Matter*, **2000**, 12, L13-L19	1.8	138
11	Al Dimer Dynamics on Al(111). *Physical Review Letters*, **1998**, 81, 172-175	7.4	51
10	Phonon superlattice transport. *Physical Review B*, **1997**, 56, 10754-10757	3.3	184
9	Electron-electron scattering in far-infrared quantum cascade lasers. *Physical Review B*, **1996**, 53, 6889-6892	3.3	45
8	Resonant Tunneling with an Electron-Phonon Interaction. *Annals of Physics*, **1994**, 236, 1-42	2.5	61
7	Current and rate equation for resonant tunneling. *Physical Review B*, **1993**, 47, 4603-4618	3.3	58
6	Zero-frequency current noise for the double-tunnel-junction Coulomb blockade. *Physical Review B*, **1993**, 47, 1967-1979	3.3	144
5	Noise as a diagnostic of tunneling mechanisms. *Physica Scripta*, **1992**, T42, 115-121	2.6	15
4	Classical theory for shot noise in resonant tunneling. *Physical Review B*, **1992**, 46, 9620-9633	3.3	108
3	Elastic and Inelastic Resonant Tunneling in an Imperfect Superlattice. *NATO ASI Series Series B: Physics*, **1991**, 535-537		
2	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	11
1	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	2.6	14