Elsebeth SchrÃ¶der

List of Publications by Year
in descending order

62 papers	9,491 citations	147801 31 h-index	123424 61 g-index
63 all docs	63 docs citations	63 times ranked	10482 citing authors

#	Article	IF	Citations
1	Van der Waals Density Functional for General Geometries. Physical Review Letters, 2004, 92, 246401.	7.8	4,707
2	Van der Waals Density Functional for Layered Structures. Physical Review Letters, 2003, 91, 126402.	7.8	623
3	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
4	Application of van der Waals Density Functional to an Extended System: Adsorption of Benzene and Naphthalene on Graphite. Physical Review Letters, 2006, 96, 146107.	7.8	382
5	A density functional for sparse matter. Journal of Physics Condensed Matter, 2009, 21, 084203.	1.8	363
6	Van der Waals density functional theory with applications. International Journal of Quantum Chemistry, 2005, 101, 599-610.	2.0	304
7	Spin Signature of Nonlocal Correlation Binding in Metal-Organic Frameworks. Physical Review Letters, 2015, 115, 136402.	7.8	272
8	Stacking Interactions and the Twist of DNA. Journal of the American Chemical Society, 2008, 130, 1304-1308.	13.7	181
9	Potassium intercalation in graphite: A van der Waals density-functional study. Physical Review B, 2007, 76, .	3.2	155
10	Towards a working density-functional theory for polymers: First-principles determination of the polyethylene crystal structure. Physical Review B, 2007, 76, .	3.2	108
11	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
12	Adsorption of phenol on graphite(0001) andÎ±â˜Al2O3(0001): Nature of van der Waals bonds from first-principles calculations. Physical Review B, 2006, 74, .	3.2	89
13	Physisorption of nucleobases on graphene: a comparative van der Waals study. Journal of Physics Condensed Matter, 2012, 24, 424210.	1.8	83
14	Role of van der Waals bonding in the layered oxide<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>V</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mtext> First-principles density-functional calculations. Physical Review B, 2010, 82, .	3.2	78
15	First-principles study of the adsorption of methanol at the Î±-Al2O3(0001) surface. Journal of Physics Condensed Matter, 2006, 18, 1-12.	1.8	65
16	Interpretation of van der Waals density functionals. Physical Review B, 2014, 90, .	3.2	63
17	Hydrogen dynamics in magnesium and graphite. Computational Materials Science, 2002, 24, 273-277.	3.0	58
18	Binding of polycyclic aromatic hydrocarbons and graphene dimers in density functional theory. New Journal of Physics, 2010, 12, 013017.	2.9	55

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19	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
20	van der Waals interactions of polycyclic aromatic hydrocarbon dimers. Journal of Chemical Physics, 2005, 122, 054102.	3.0	46
21	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
22	A van der Waals density functional study of adenine on graphene: single-molecular adsorption and overlayer binding. Journal of Physics Condensed Matter, 2011, 23, 135001.	1.8	44
23	Vanadium pentoxide (V2O5): A van der Waals density functional study. Computer Physics Communications, 2011, 182, 1805-1809.	7.5	44
24	Theory for structure and bulk modulus determination. Physical Review B, 2003, 68, .	3.2	42
25	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
26	Methanol Adsorption on Graphene. Journal of Nanomaterials, 2013, 2013, 1-6.	2.7	35
27	Adsorption of methylamine onÎ±â^'Al2O3(0001)andÎ±â^'Cr2O3(0001): Density functional theory. Physical Review B, 2007, 75, .	3.2	34
28	Van der Waals interactions of parallel and concentric nanotubes. Materials Science and Engineering C, 2003, 23, 721-725.	7.3	33
29	O adsorption and incipient oxidation of the Mg(0001) surface. Physical Review B, 2004, 69, .	3.2	33
30	A Mechanism for Highly Efficient Electrochemical Bubbling Delamination of CVDâ€Grown Graphene from Metal Substrates. Advanced Materials Interfaces, 2016, 3, 1500492.	3.7	33
31	Vortex Dynamics in Dissipative Systems. Physical Review Letters, 1997, 78, 1908-1911.	7.8	32
32	Density-functional bridge between surfaces and interfaces. Surface Science, 2001, 493, 253-270.	1.9	31
33	Desorption of n-alkanes from graphene: a van der Waals density functional study. Journal of Physics Condensed Matter, 2012, 24, 424212.	1.8	27
34	Relative Particle Motion in Capillary Waves. Physical Review Letters, 1996, 76, 4717-4720.	7.8	25
35	Fractal Particle Trajectories in Capillary Waves: Imprint of Wavelength. Physical Review Letters, 1997, 79, 1845-1848.	7.8	25
36	A van der Waals density functional study of chloroform and other trihalomethanes on graphene. Journal of Chemical Physics, 2012, 137, 174702.	3.0	25

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37	van der Waals interaction of simple, parallel polymers. Journal of Chemical Physics, 2005, 122, 164902.	3.0	24
38	Van der Waals interaction of parallel polymers and nanotubes. Computational Materials Science, 2005, 33, 192-199.	3.0	22
39	Adsorption of methanol and methoxy on the Î±-Cr2O3(0001) surface. Journal of Physics Condensed Matter, 2006, 18, 10751-10763.	1.8	19
40	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
41	Mg(0001) surface oxidation: A two-dimensional oxide phase. Physical Review B, 2004, 69, .	3.2	18
42	Signatures of van der Waals binding: A coupling-constant scaling analysis. Physical Review B, 2018, 97, .	3.2	17
43	Extent of Fock-exchange mixing for a hybrid van der Waals density functional?. Journal of Chemical Physics, 2018, 148, 194115.	3.0	17
44	van der Waals interactions of the benzene dimer: Towards treatment of polycyclic aromatic hydrocarbon dimers. Materials Science and Engineering C, 2005, 25, 787-792.	7.3	16
45	Graphene oxide and adsorption of chloroform: A density functional study. Journal of Chemical Physics, 2016, 144, 184704.	3.0	15
46	Methylbenzenes on graphene. Surface Science, 2017, 664, 162-167.	1.9	15
47	The van der Waals interactions of concentric nanotubes. Surface Science, 2003, 532-535, 880-885.	1.9	14
48	Ab initioinvestigation of monoclinic phase stability and martensitic transformation in crystalline polyethylene. Physical Review Materials, 2018, 2, .	2.4	14
49	Nematic liquid-crystal director configuration for general elastic coefficients. Physical Review E, 2000, 62, 8830-8833.	2.1	11
50	Ultrathin Pd and Pt films on W(211). Thin Solid Films, 2003, 428, 47-51.	1.8	11
51	Filter function of graphene oxide: Trapping perfluorinated molecules. Journal of Chemical Physics, 2020, 152, 024704.	3.0	9
52	Untwinned <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>YBa</mml:mi><mml:mn>2</mml:mn></mml mathvariant="normal">O</mml:mi><mml:mrow><mml:mn>7</mml:mn><mml:mo>â^'</mml:mo><mml:mi>Î´</mml:mi></mml:mrow></ thin films on MgO substrates: A platform to study strain effects on the local orders in cuprates. Physical Review Materials, 2019, 3, .	2.4	9
53	Harris-type van der Waals density functional scheme. Physical Review B, 2013, 88, .	3.2	8
54	The vdW-DF Family of Nonlocal Exchange-Correlation Functionals. , 2017, , 241-274.		8

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55	Velocity correlations in weakly turbulent surface waves. Physical Review E, 1998, 57, 7329-7331.	2.1	7
56	Interaction effects in magnesium oxidation: a lattice-gas simulation. Computational Materials Science, 2002, 24, 105-110.	3.0	7
57	Self-diffusion and relative diffusion in defect turbulence. Physica D: Nonlinear Phenomena, 1996, 96, 1-8.	2.8	6
58	Bridging between micro- and macroscales of materials by mesoscopic models. Computational Materials Science, 2002, 24, 1-13.	3.0	4
59	Hard and soft materials: putting consistent van der Waals density functionals to work. Electronic Structure, 2022, 4, 014001.	2.8	4
60	Fractional Brownian motion of particles in capillary waves. Physica A: Statistical Mechanics and Its Applications, 1997, 239, 314-321.	2.6	2
61	Involving High School Students in Computational Physics University Research: Theory Calculations of Toluene Adsorbed on Graphene. PLoS ONE, 2016, 11, e0159168.	2.5	2
62	Toward a String Formulation of Vortex Dynamics. , 2000, , 263-267.		0