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	Hard and soft materials: putting consistent van der Waals density functionals to work. Electronic Structure, 2022, 4, 014001.	2.8	4
2	Filter function of graphene oxide: Trapping perfluorinated molecules. Journal of Chemical Physics, 2020, 152, 024704.	3.0	9
3	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:msub><mml:msub><mml:mi>Cu</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi>O</mml:mi><mml:mrow><mml:mn>7</mml:mn><mml:mo>−</mml:mo><mml:mi>δ</mml:mi></mml:mrow></mml:msub></mml:mrow></mml:math> 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
4	Signatures of van der Waals binding: A coupling-constant scaling analysis. Physical Review B, 2018, 97, .	3.2	17
5	Extent of Fock-exchange mixing for a hybrid van der Waals density functional?. Journal of Chemical Physics, 2018, 148, 194115.	3.0	17
6	Ab initioinvestigation of monoclinic phase stability and martensitic transformation in crystalline polyethylene. Physical Review Materials, 2018, 2, .	2.4	14
7	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
8	Methylbenzenes on graphene. Surface Science, 2017, 664, 162-167.	1.9	15
9	The vdW-DF Family of Nonlocal Exchange-Correlation Functionals. , 2017, , 241-274.		8
10	A Mechanism for Highly Efficient Electrochemical Bubbling Delamination of CVDâ€Grown Graphene from Metal Substrates. Advanced Materials Interfaces, 2016, 3, 1500492.	3.7	33
11	Graphene oxide and adsorption of chloroform: A density functional study. Journal of Chemical Physics, 2016, 144, 184704.	3.0	15
12	Involving High School Students in Computational Physics University Research: Theory Calculations of Toluene Adsorbed on Graphene. PLoS ONE, 2016, 11, e0159168.	2.5	2
13	Spin Signature of Nonlocal Correlation Binding in Metal-Organic Frameworks. Physical Review Letters, 2015, 115, 136402.	7.8	272
14	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
15	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
16	Interpretation of van der Waals density functionals. Physical Review B, 2014, 90, .	3.2	63
17	Methanol Adsorption on Graphene. Journal of Nanomaterials, 2013, 2013, 1-6.	2.7	35
18	Harris-type van der Waals density functional scheme. Physical Review B, 2013, 88, .	3.2	8

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19	Physisorption of nucleobases on graphene: a comparative van der Waals study. Journal of Physics Condensed Matter, 2012, 24, 424210.	1.8	83
20	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
21	Desorption of n-alkanes from graphene: a van der Waals density functional study. Journal of Physics Condensed Matter, 2012, 24, 424212.	1.8	27
22	A van der Waals density functional study of chloroform and other trihalomethanes on graphene. Journal of Chemical Physics, 2012, 137, 174702.	3.0	25
23	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
24	Vanadium pentoxide (V2O5): A van der Waals density functional study. Computer Physics Communications, 2011, 182, 1805-1809.	7.5	44
25	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
26	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
27	Binding of polycyclic aromatic hydrocarbons and graphene dimers in density functional theory. New Journal of Physics, 2010, 12, 013017.	2.9	55
28	A density functional for sparse matter. Journal of Physics Condensed Matter, 2009, 21, 084203.	1.8	363
29	Stacking Interactions and the Twist of DNA. Journal of the American Chemical Society, 2008, 130, 1304-1308.	13.7	181
30	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
31	Adsorption of methylamine onÎ±â^'Al2O3(0001)andÎ±â^'Cr2O3(0001): Density functional theory. Physical Review B, 2007, 75, .	3.2	34
32	Towards a working density-functional theory for polymers: First-principles determination of the polyethylene crystal structure. Physical Review B, 2007, 76, .	3.2	108
33	Potassium intercalation in graphite: A van der Waals density-functional study. Physical Review B, 2007, 76, .	3.2	155
34	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
35	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
36	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

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37	Adsorption of methanol and methoxy on the Î±-Cr2O3(0001) surface. Journal of Physics Condensed Matter, 2006, 18, 10751-10763.	1.8	19
38	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
39	Van der Waals density functional theory with applications. International Journal of Quantum Chemistry, 2005, 101, 599-610.	2.0	304
40	van der Waals interaction of simple, parallel polymers. Journal of Chemical Physics, 2005, 122, 164902.	3.0	24
41	Van der Waals interaction of parallel polymers and nanotubes. Computational Materials Science, 2005, 33, 192-199.	3.0	22
42	van der Waals interactions of polycyclic aromatic hydrocarbon dimers. Journal of Chemical Physics, 2005, 122, 054102.	3.0	46
43	O adsorption and incipient oxidation of the Mg(0001) surface. Physical Review B, 2004, 69, .	3.2	33
44	Mg(0001) surface oxidation: A two-dimensional oxide phase. Physical Review B, 2004, 69, .	3.2	18
45	Van der Waals Density Functional for General Geometries. Physical Review Letters, 2004, 92, 246401.	7.8	4,707
46	Theory for structure and bulk modulus determination. Physical Review B, 2003, 68, .	3.2	42
47	Van der Waals Density Functional for Layered Structures. Physical Review Letters, 2003, 91, 126402.	7.8	623
48	Van der Waals interactions of parallel and concentric nanotubes. Materials Science and Engineering C, 2003, 23, 721-725.	7.3	33
49	Ultrathin Pd and Pt films on W(211). Thin Solid Films, 2003, 428, 47-51.	1.8	11
50	The van der Waals interactions of concentric nanotubes. Surface Science, 2003, 532-535, 880-885.	1.9	14
51	Bridging between micro- and macroscales of materials by mesoscopic models. Computational Materials Science, 2002, 24, 1-13.	3.0	4
52	Interaction effects in magnesium oxidation: a lattice-gas simulation. Computational Materials Science, 2002, 24, 105-110.	3.0	7
53	Hydrogen dynamics in magnesium and graphite. Computational Materials Science, 2002, 24, 273-277.	3.0	58
54	Density-functional bridge between surfaces and interfaces. Surface Science, 2001, 493, 253-270.	1.9	31

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55	Nematic liquid-crystal director configuration for general elastic coefficients. Physical Review E, 2000, 62, 8830-8833.	2.1	11
56	Toward a String Formulation of Vortex Dynamics. , 2000, , 263-267.		0
57	Velocity correlations in weakly turbulent surface waves. Physical Review E, 1998, 57, 7329-7331.	2.1	7
58	Vortex Dynamics in Dissipative Systems. Physical Review Letters, 1997, 78, 1908-1911.	7.8	32
59	Fractal Particle Trajectories in Capillary Waves: Imprint of Wavelength. Physical Review Letters, 1997, 79, 1845-1848.	7.8	25
60	Fractional Brownian motion of particles in capillary waves. Physica A: Statistical Mechanics and Its Applications, 1997, 239, 314-321.	2.6	2
61	Self-diffusion and relative diffusion in defect turbulence. Physica D: Nonlinear Phenomena, 1996, 96, 1-8.	2.8	6
62	Relative Particle Motion in Capillary Waves. Physical Review Letters, 1996, 76, 4717-4720.	7.8	25