

Jiri Klimes

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

39
papers

7,711
citations

28
h-index

41
g-index

41
ext. papers

8,538
ext. citations

5.3
avg, IF

6.48
L-index

#	Paper	IF	Citations
39	Van der Waals density functionals applied to solids. <i>Physical Review B</i> , 2011 , 83,	3.3	2972
38	Chemical accuracy for the van der Waals density functional. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 022201	1.8	1759
37	Perspective: Advances and challenges in treating van der Waals dispersion forces in density functional theory. <i>Journal of Chemical Physics</i> , 2012 , 137, 120901	3.9	813
36	Graphene on Ni(111): Strong interaction and weak adsorption. <i>Physical Review B</i> , 2011 , 84,	3.3	218
35	Hydrogen bonds and van der waals forces in ice at ambient and high pressures. <i>Physical Review Letters</i> , 2011 , 107, 185701	7.4	181
34	The role of van der Waals forces in water adsorption on metals. <i>Journal of Chemical Physics</i> , 2013 , 138, 024708	3.9	155
33	To wet or not to wet? Dispersion forces tip the balance for water ice on metals. <i>Physical Review Letters</i> , 2011 , 106, 026101	7.4	151
32	Predictive GW calculations using plane waves and pseudopotentials. <i>Physical Review B</i> , 2014 , 90,	3.3	135
31	Improved description of soft layered materials with van der Waals density functional theory. <i>Journal of Physics Condensed Matter</i> , 2012 , 24, 424216	1.8	134
30	On the accuracy of van der Waals inclusive density-functional theory exchange-correlation functionals for ice at ambient and high pressures. <i>Journal of Chemical Physics</i> , 2013 , 139, 154702	3.9	107
29	Cubic scaling algorithm for the random phase approximation: Self-interstitials and vacancies in Si. <i>Physical Review B</i> , 2014 , 90,	3.3	104
28	Low Scaling Algorithms for the Random Phase Approximation: Imaginary Time and Laplace Transformations. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 2498-507	6.4	88
27	Lattice constants and cohesive energies of alkali, alkaline-earth, and transition metals: Random phase approximation and density functional theory results. <i>Physical Review B</i> , 2013 , 87,	3.3	85
26	Cubic scaling GW: Towards fast quasiparticle calculations. <i>Physical Review B</i> , 2016 , 94,	3.3	74
25	Influence of water on the electronic structure of metal-supported graphene: Insights from van der Waals density functional theory. <i>Physical Review B</i> , 2012 , 85,	3.3	61
24	Proton ordering in cubic ice and hexagonal ice; a potential new ice phase-XIc. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 19788-95	3.6	55
23	Understanding the interaction of the porphyrin macrocycle to reactive metal substrates: structure, bonding, and adatom capture. <i>ACS Nano</i> , 2011 , 5, 1831-8	16.7	55

22	Vibronic Effects in Single Molecule Conductance: First-Principles Description and Application to Benzenealkanethiolates between Gold Electrodes. <i>Journal of Physical Chemistry C</i> , 2008 , 112, 9880-9890 ^{3.8}	3.8	54
21	Fast and accurate quantum Monte Carlo for molecular crystals. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018 , 115, 1724-1729	11.5	52
20	A critical assessment of theoretical methods for finding reaction pathways and transition states of surface processes. <i>Journal of Physics Condensed Matter</i> , 2010 , 22, 074203	1.8	49
19	The accurate calculation of the band gap of liquid water by means of GW corrections applied to plane-wave density functional theory molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , 2015 , 17, 365-75	3.6	46
18	The random phase approximation applied to ice. <i>Journal of Chemical Physics</i> , 2014 , 140, 084502	3.9	40
17	Kohn-Sham band gaps and potentials of solids from the optimised effective potential method within the random phase approximation. <i>Journal of Chemical Physics</i> , 2014 , 140, 054516	3.9	40
16	Cooperative interplay of van der Waals forces and quantum nuclear effects on adsorption: H at graphene and at coronene. <i>ACS Nano</i> , 2014 , 8, 9905-13	16.7	38
15	Trends in water monomer adsorption and dissociation on flat insulating surfaces. <i>Physical Chemistry Chemical Physics</i> , 2011 , 13, 12447-53	3.6	38
14	Beyond the quasiparticle approximation: Fully self-consistent GW calculations. <i>Physical Review B</i> , 2018 , 98,	3.3	35
13	Understanding the role of ions and water molecules in the NaCl dissolution process. <i>Journal of Chemical Physics</i> , 2013 , 139, 234702	3.9	34
12	Singles correlation energy contributions in solids. <i>Journal of Chemical Physics</i> , 2015 , 143, 102816	3.9	29
11	Proton transfer in adsorbed water dimers. <i>Physical Chemistry Chemical Physics</i> , 2010 , 12, 3953-6	3.6	28
10	Lattice energies of molecular solids from the random phase approximation with singles corrections. <i>Journal of Chemical Physics</i> , 2016 , 145, 094506	3.9	22
9	Temperature Dependence of Carbon Monoxide Adsorption on a High-Silica H-FER Zeolite. <i>Journal of Physical Chemistry C</i> , 2018 , 122, 26088-26095	3.8	11
8	Increase in Solubility of Poorly-Ionizable Pharmaceuticals by Salt Formation: A Case of Agomelatine Sulfonates. <i>Crystal Growth and Design</i> , 2017 , 17, 5283-5294	3.5	9
7	The nature of bonding and electronic properties of graphene and benzene with iridium adatoms. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 20818-27	3.6	8
6	Random Phase Approximation Applied to Many-Body Noncovalent Systems. <i>Journal of Chemical Theory and Computation</i> , 2020 , 16, 427-442	6.4	7
5	Efficient and accurate description of adsorption in zeolites. <i>Journal of Chemical Physics</i> , 2019 , 151, 234108	3.9	7

4	Anomalous Freezing of Low-Dimensional Water Confined in Graphene Nanowrinkles. <i>ACS Nano</i> , 2020 , 14, 15587-15594	16.7	6
3	Ferroelectric 2D ice under graphene confinement. <i>Nature Communications</i> , 2021 , 12, 6291	17.4	3
2	Insights on hydrogen bond assisted solvent selection in certain acidBase heterogeneous catalysis through acceptor and donor numbers. <i>Catalysis Science and Technology</i> , 2021 , 11, 1345-1357	5.5	3
1	Random-Phase Approximation in Many-Body Noncovalent Systems: Methane in a Dodecahedral Water Cage. <i>Journal of Chemical Theory and Computation</i> , 2021 , 17, 804-817	6.4	3