Jiri Klimes

List of Publications by Year in Descending Order

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	Ferroelectric 2D ice under graphene confinement. *Nature Communications*, **2021**, 12, 6291	17.4	3
38	Insights on hydrogen bond assisted solvent selection in certain acid–base heterogeneous catalysis through acceptor and donor numbers. *Catalysis Science and Technology*, **2021**, 11, 1345-1357	5.5	3
37	Random-Phase Approximation in Many-Body Noncovalent Systems: Methane in a Dodecahedral Water Cage. *Journal of Chemical Theory and Computation*, **2021**, 17, 804-817	6.4	3
36	Random Phase Approximation Applied to Many-Body Noncovalent Systems. *Journal of Chemical Theory and Computation*, **2020**, 16, 427-442	6.4	7
35	Anomalous Freezing of Low-Dimensional Water Confined in Graphene Nanowrinkles. *ACS Nano*, **2020**, 14, 15587-15594	16.7	6
34	Efficient and accurate description of adsorption in zeolites. *Journal of Chemical Physics*, **2019**, 151, 234108	3.9	7
33	Fast and accurate quantum Monte Carlo for molecular crystals. *Proceedings of the National Academy of Sciences of the United States of America*, **2018**, 115, 1724-1729	11.5	52
32	Temperature Dependence of Carbon Monoxide Adsorption on a High-Silica H-FER Zeolite. *Journal of Physical Chemistry C*, **2018**, 122, 26088-26095	3.8	11
31	Beyond the quasiparticle approximation: Fully self-consistent GW calculations. *Physical Review B*, **2018**, 98,	3.3	35
30	Increase in Solubility of Poorly-Ionizable Pharmaceuticals by Salt Formation: A Case of Agomelatine Sulfonates. *Crystal Growth and Design*, **2017**, 17, 5283-5294	3.5	9
29	Lattice energies of molecular solids from the random phase approximation with singles corrections. *Journal of Chemical Physics*, **2016**, 145, 094506	3.9	22
28	Cubic scaling GW: Towards fast quasiparticle calculations. *Physical Review B*, **2016**, 94,	3.3	74
27	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. *Physical Chemistry Chemical Physics*, **2015**, 17, 365-75	3.6	46
26	Singles correlation energy contributions in solids. *Journal of Chemical Physics*, **2015**, 143, 102816	3.9	29
25	Cooperative interplay of van der Waals forces and quantum nuclear effects on adsorption: H at graphene and at coronene. *ACS Nano*, **2014**, 8, 9905-13	16.7	38
24	Low Scaling Algorithms for the Random Phase Approximation: Imaginary Time and Laplace Transformations. *Journal of Chemical Theory and Computation*, **2014**, 10, 2498-507	6.4	88
23	The nature of bonding and electronic properties of graphene and benzene with iridium adatoms. *Physical Chemistry Chemical Physics*, **2014**, 16, 20818-27	3.6	8

22	The random phase approximation applied to ice. *Journal of Chemical Physics*, **2014**, 140, 084502	3.9	40
21	Predictive GW calculations using plane waves and pseudopotentials. *Physical Review B*, **2014**, 90,	3.3	135
20	Kohn-Sham band gaps and potentials of solids from the optimised effective potential method within the random phase approximation. *Journal of Chemical Physics*, **2014**, 140, 054516	3.9	40
19	Cubic scaling algorithm for the random phase approximation: Self-interstitials and vacancies in Si. *Physical Review B*, **2014**, 90,	3.3	104
18	Lattice constants and cohesive energies of alkali, alkaline-earth, and transition metals: Random phase approximation and density functional theory results. *Physical Review B*, **2013**, 87,	3.3	85
17	The role of van der Waals forces in water adsorption on metals. *Journal of Chemical Physics*, **2013**, 138, 024708	3.9	155
16	Understanding the role of ions and water molecules in the NaCl dissolution process. *Journal of Chemical Physics*, **2013**, 139, 234702	3.9	34
15	On the accuracy of van der Waals inclusive density-functional theory exchange-correlation functionals for ice at ambient and high pressures. *Journal of Chemical Physics*, **2013**, 139, 154702	3.9	107
14	Influence of water on the electronic structure of metal-supported graphene: Insights from van der Waals density functional theory. *Physical Review B*, **2012**, 85,	3.3	61
13	Perspective: Advances and challenges in treating van der Waals dispersion forces in density functional theory. *Journal of Chemical Physics*, **2012**, 137, 120901	3.9	813
12	Improved description of soft layered materials with van der Waals density functional theory. *Journal of Physics Condensed Matter*, **2012**, 24, 424216	1.8	134
11	Graphene on Ni(111): Strong interaction and weak adsorption. *Physical Review B*, **2011**, 84,	3.3	218
10	Van der Waals density functionals applied to solids. *Physical Review B*, **2011**, 83,	3.3	2972
9	Trends in water monomer adsorption and dissociation on flat insulating surfaces. *Physical Chemistry Chemical Physics*, **2011**, 13, 12447-53	3.6	38
8	To wet or not to wet? Dispersion forces tip the balance for water ice on metals. *Physical Review Letters*, **2011**, 106, 026101	7.4	151
7	Proton ordering in cubic ice and hexagonal ice; a potential new ice phase--XIc. *Physical Chemistry Chemical Physics*, **2011**, 13, 19788-95	3.6	55
6	Hydrogen bonds and van der waals forces in ice at ambient and high pressures. *Physical Review Letters*, **2011**, 107, 185701	7.4	181
5	Understanding the interaction of the porphyrin macrocycle to reactive metal substrates: structure, bonding, and adatom capture. *ACS Nano*, **2011**, 5, 1831-8	16.7	55

4	A critical assessment of theoretical methods for finding reaction pathways and transition states of surface processes. *Journal of Physics Condensed Matter*, **2010**, 22, 074203	1.8	49
3	Chemical accuracy for the van der Waals density functional. *Journal of Physics Condensed Matter*, **2010**, 22, 022201	1.8	1759
2	Proton transfer in adsorbed water dimers. *Physical Chemistry Chemical Physics*, **2010**, 12, 3953-6	3.6	28
1	Vibronic Effects in Single Molecule Conductance: First-Principles Description and Application to Benzenealkanethiolates between Gold Electrodes. *Journal of Physical Chemistry C*, **2008**, 112, 9880-9890	3.8	54