Matthias S Rupp

List of Publications by Citations

44 papers	5,167 citations	27 h-index	47 g-index
47 ext. papers	6,132 ext. citations	4.9 avg, IF	6.03 L-index

#	Paper	IF	Citations
44	Fast and accurate modeling of molecular atomization energies with machine learning. *Physical Review Letters*, **2012**, 108, 058301	7.4	1099
43	Quantum chemistry structures and properties of 134 kilo molecules. *Scientific Data*, **2014**, 1, 140022	8.2	514
42	Assessment and Validation of Machine Learning Methods for Predicting Molecular Atomization Energies. *Journal of Chemical Theory and Computation*, **2013**, 9, 3404-19	6.4	410
41	Finding density functionals with machine learning. *Physical Review Letters*, **2012**, 108, 253002	7.4	400
40	Big Data Meets Quantum Chemistry Approximations: The Machine Learning Approach. *Journal of Chemical Theory and Computation*, **2015**, 11, 2087-96	6.4	382
39	Machine learning of molecular electronic properties in chemical compound space. *New Journal of Physics*, **2013**, 15, 095003	2.9	366
38	Online chemical modeling environment (OCHEM): web platform for data storage, model development and publishing of chemical information. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 533-54	4.2	311
37	Machine learning for quantum mechanics in a nutshell. *International Journal of Quantum Chemistry*, **2015**, 115, 1058-1073	2.1	217
36	Fourier series of atomic radial distribution functions: A molecular fingerprint for machine learning models of quantum chemical properties. *International Journal of Quantum Chemistry*, **2015**, 115, 1084-1093	2.1	153
35	DOGS: reaction-driven de novo design of bioactive compounds. *PLoS Computational Biology*, **2012**, 8, e1002380	5	151
34	Machine Learning for Quantum Mechanical Properties of Atoms in Molecules. *Journal of Physical Chemistry Letters*, **2015**, 6, 3309-3313	6.4	132
33	Understanding machine-learned density functionals. *International Journal of Quantum Chemistry*, **2016**, 116, 819-833	2.1	98
32	Modeling of molecular atomization energies using machine learning. *Journal of Cheminformatics*, **2012**, 4,	8.6	78
31	Graph kernels for chemoinformatics a critical discussion. *Journal of Cheminformatics*, **2011**, 3,	8.6	78
30	Orbital-free bond breaking via machine learning. *Journal of Chemical Physics*, **2013**, 139, 224104	3.9	74
29	Optimizing transition states via kernel-based machine learning. *Journal of Chemical Physics*, **2012**, 136, 174101	3.9	74
28	Understanding kernel ridge regression: Common behaviors from simple functions to density functionals. *International Journal of Quantum Chemistry*, **2015**, 115, 1115-1128	2.1	65

27	Kernel approach to molecular similarity based on iterative graph similarity. *Journal of Chemical Information and Modeling*, **2007**, 47, 2280-6	6.1	54
26	From machine learning to natural product derivatives that selectively activate transcription factor PPARgamma. *ChemMedChem*, **2010**, 5, 191-4	3.7	47
25	Machine-learned multi-system surrogate models for materials prediction. *Npj Computational Materials*, **2019**, 5,	10.9	42
24	Visual Interpretation of Kernel-Based Prediction Models. *Molecular Informatics*, **2011**, 30, 817-26	3.8	40
23	Predicting the pKa of small molecule. *Combinatorial Chemistry and High Throughput Screening*, **2011**, 14, 307-27	1.3	36
22	Shapelets: possibilities and limitations of shape-based virtual screening. *Journal of Computational Chemistry*, **2008**, 29, 108-14	3.5	29
21	Identifying domains of applicability of machine learning models for materials science. *Nature Communications*, **2020**, 11, 4428	17.4	29
20	Graph Kernels for Molecular Similarity. *Molecular Informatics*, **2010**, 29, 266-73	3.8	28
19	Chemical diversity in molecular orbital energy predictions with kernel ridge regression. *Journal of Chemical Physics*, **2019**, 150, 204121	3.9	27
18	Machine learning estimates of natural product conformational energies. *PLoS Computational Biology*, **2014**, 10, e1003400	5	26
17	Distance phenomena in high-dimensional chemical descriptor spaces: consequences for similarity-based approaches. *Journal of Computational Chemistry*, **2009**, 30, 2285-96	3.5	20
16	Rupp et al. Reply:. *Physical Review Letters*, **2012**, 109,	7.4	20
15	Nonlinear gradient denoising: Finding accurate extrema from inaccurate functional derivatives. *International Journal of Quantum Chemistry*, **2015**, 115, 1102-1114	2.1	18
14	Estimation of Acid Dissociation Constants Using Graph Kernels. *Molecular Informatics*, **2010**, 29, 731-40	3.8	15
13	Assessing the frontier: Active learning, model accuracy, and multi-objective candidate discovery and optimization. *Journal of Chemical Physics*, **2020**, 153, 024112	3.9	14
12	Special issue on machine learning and quantum mechanics. *International Journal of Quantum Chemistry*, **2015**, 115, 1003-1004	2.1	12
11	Truxillic acid derivatives act as peroxisome proliferator-activated receptor gamma activators. *Bioorganic and Medicinal Chemistry Letters*, **2010**, 20, 2920-3	2.9	9
10	Target Profile Prediction: Cross-Activation of Peroxisome Proliferator-Activated Receptor (PPAR) and Farnesoid X Receptor (FXR). *Molecular Informatics*, **2010**, 29, 287-92	3.8	8

9	Pharmacophore alignment search tool: Influence of canonical atom labeling on similarity searching. *Journal of Computational Chemistry*, **2010**, 31, 2810-26	3.5	7
8	Spherical harmonics coefficients for ligand-based virtual screening of cyclooxygenase inhibitors. *PLoS ONE*, **2011**, 6, e21554	3.7	6
7	Impact of X-Ray Structure on Predictivity of Scoring Functions: PPAR Case Study. *Molecular Informatics*, **2012**, 31, 631-3	3.8	5
6	Multi-task learning for pKa prediction. *Journal of Computer-Aided Molecular Design*, **2012**, 26, 883-95	4.2	5
5	Representations of molecules and materials for interpolation of quantum-mechanical simulations via machine learning. *Npj Computational Materials*, **2022**, 8,	10.9	4
4	Pharmacophore Alignment Search Tool (PhAST): Significance Assessment of Chemical Similarity. *Molecular Informatics*, **2013**, 32, 625-46	3.8	2
3	Kernel learning for ligand-based virtual screening: discovery of a new PPAR agonist. *Journal of Cheminformatics*, **2010**, 2,	8.6	2
2	Identifying Domains of Applicability of Machine Learning Models for Materials Science		2
1	Graph Kernels217-243		1