Matthias S Rupp

List of Publications by Year
in descending order

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43 papers	7,013 citations	212478 28 h-index	286692 43 g-index
47 all docs	47 docs citations	47 times ranked	6278 citing authors

#	Article	IF	Citations
1	Representations of molecules and materials for interpolation of quantum-mechanical simulations via machine learning. Npj Computational Materials, 2022, 8, .	3.5	54
2	Identifying domains of applicability of machine learning models for materials science. Nature Communications, 2020, 11, 4428.	5.8	66
3	Assessing the frontier: Active learning, model accuracy, and multi-objective candidate discovery and optimization. Journal of Chemical Physics, 2020, 153, 024112.	1.2	34
4	Chemical diversity in molecular orbital energy predictions with kernel ridge regression. Journal of Chemical Physics, 2019, 150, 204121.	1.2	59
5	Machine-learned multi-system surrogate models for materials prediction. Npj Computational Materials, 2019, 5, .	3.5	96
6	Guest Editorial: Special Topic on Data-Enabled Theoretical Chemistry. Journal of Chemical Physics, 2018, 148, 241401.	1.2	77
7	Understanding machineâ€learned density functionals. International Journal of Quantum Chemistry, 2016, 116, 819-833.	1.0	132
8	Understanding kernel ridge regression: Common behaviors from simple functions to density functionals. International Journal of Quantum Chemistry, 2015, 115, 1115-1128.	1.0	89
9	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.	1.0	181
10	Nonlinear gradient denoising: Finding accurate extrema from inaccurate functional derivatives. International Journal of Quantum Chemistry, 2015, 115, 1102-1114.	1.0	21
11	Special issue on machine learning and quantum mechanics. International Journal of Quantum Chemistry, 2015, 115, 1003-1004.	1.0	14
12	Big Data Meets Quantum Chemistry Approximations: The Î”-Machine Learning Approach. Journal of Chemical Theory and Computation, 2015, 11, 2087-2096.	2.3	579
13	Machine learning for quantum mechanics in a nutshell. International Journal of Quantum Chemistry, 2015, 115, 1058-1073.	1.0	288
14	Machine Learning for Quantum Mechanical Properties of Atoms in Molecules. Journal of Physical Chemistry Letters, 2015, 6, 3309-3313.	2.1	169
15	Machine Learning Estimates of Natural Product Conformational Energies. PLoS Computational Biology, 2014, 10, e1003400.	1.5	30
16	Quantum chemistry structures and properties of 134 kilo molecules. Scientific Data, 2014, 1, 140022.	2.4	887
17	Assessment and Validation of Machine Learning Methods for Predicting Molecular Atomization Energies. Journal of Chemical Theory and Computation, 2013, 9, 3404-3419.	2.3	499
18	Machine learning of molecular electronic properties in chemical compound space. New Journal of Physics, 2013, 15, 095003.	1.2	482

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19	Orbital-free bond breaking via machine learning. Journal of Chemical Physics, 2013, 139, 224104.	1.2	92
20	Pharmacophore Alignment Search Tool (PhAST): Significance Assessment of Chemical Similarity. Molecular Informatics, 2013, 32, 625-646.	1.4	2
21	DOGS: Reaction-Driven de novo Design of Bioactive Compounds. PLoS Computational Biology, 2012, 8, e1002380.	1.5	193
22	Finding Density Functionals with Machine Learning. Physical Review Letters, 2012, 108, 253002.	2.9	495
23	RuppetÂal.Reply:. Physical Review Letters, 2012, 109, .	2.9	20
24	Optimizing transition states via kernel-based machine learning. Journal of Chemical Physics, 2012, 136, 174101.	1.2	92
25	Impact of Xâ€Ray Structure on Predictivity of Scoring Functions: PPARÎ³ Case Study. Molecular Informatics, 2012, 31, 631-633.	1.4	5
26	Fast and Accurate Modeling of Molecular Atomization Energies with Machine Learning. Physical Review Letters, 2012, 108, 058301.	2.9	1,523
27	Multi-task learning for pKa prediction. Journal of Computer-Aided Molecular Design, 2012, 26, 883-895.	1.3	7
28	Modeling of molecular atomization energies using machine learning. Journal of Cheminformatics, 2012, 4, .	2.8	2
29	Spherical Harmonics Coefficients for Ligand-Based Virtual Screening of Cyclooxygenase Inhibitors. PLoS ONE, 2011, 6, e21554.	1.1	8
30	Predicting the pKa of Small Molecules. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 307-327.	0.6	50
31	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, 533-554.	1.3	453
32	Graph kernels for chemoinformatics â€“ a critical discussion. Journal of Cheminformatics, 2011, 3, .	2.8	2
33	Visual Interpretation of Kernelâ€Based Prediction Models. Molecular Informatics, 2011, 30, 817-826.	1.4	46
34	From Machine Learning to Natural Product Derivatives that Selectively Activate Transcription Factor PPARÎ³. ChemMedChem, 2010, 5, 191-194.	1.6	58
35	Pharmacophore alignment search tool: Influence of canonical atom labeling on similarity searching. Journal of Computational Chemistry, 2010, 31, 2810-2826.	1.5	8
36	Target Profile Prediction: Crossâ€Activation of Peroxisome Proliferatorâ€Activated Receptor (PPAR) and Farnesoid X Receptor (FXR). Molecular Informatics, 2010, 29, 287-292.	1.4	8

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37	Graph Kernels for Molecular Similarity. Molecular Informatics, 2010, 29, 266-273.	1.4	35
38	Estimation of Acid Dissociation Constants Using Graph Kernels. Molecular Informatics, 2010, 29, 731-740.	1.4	23
39	Truxillic acid derivatives act as peroxisome proliferator-activated receptor Î³ activators. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 2920-2923.	1.0	11
40	Kernel learning for ligand-based virtual screening: discovery of a new PPARÎ³ agonist. Journal of Cheminformatics, 2010, 2, .	2.8	2
41	Distance phenomena in highâ€dimensional chemical descriptor spaces: Consequences for similarityâ€based approaches. Journal of Computational Chemistry, 2009, 30, 2285-2296.	1.5	21
42	Shapelets: Possibilities and limitations of shape-based virtual screening. Journal of Computational Chemistry, 2008, 29, 108-114.	1.5	32
43	Kernel Approach to Molecular Similarity Based on Iterative Graph Similarity. Journal of Chemical Information and Modeling, 2007, 47, 2280-2286.	2.5	64