Raghunathan Ramakrishnan

List of Publications by Citations

28 papers	2,055 citations	14 h-index	34 g-index
34 ext. papers	2,473 ext. citations	4.3 avg, IF	5.34 L-index

#	Paper	IF	Citations
28	Quantum chemistry structures and properties of 134 kilo molecules. *Scientific Data*, **2014**, 1, 140022	8.2	514
27	Machine Learning Predictions of Molecular Properties: Accurate Many-Body Potentials and Nonlocality in Chemical Space. *Journal of Physical Chemistry Letters*, **2015**, 6, 2326-31	6.4	426
26	Big Data Meets Quantum Chemistry Approximations: The Machine Learning Approach. *Journal of Chemical Theory and Computation*, **2015**, 11, 2087-96	6.4	382
25	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
24	Machine Learning for Quantum Mechanical Properties of Atoms in Molecules. *Journal of Physical Chemistry Letters*, **2015**, 6, 3309-3313	6.4	132
23	Electronic spectra from TDDFT and machine learning in chemical space. *Journal of Chemical Physics*, **2015**, 143, 084111	3.9	114
22	Many Molecular Properties from One Kernel in Chemical Space. *Chimia*, **2015**, 69, 182-6	1.3	59
21	Genetic Optimization of Training Sets for Improved Machine Learning Models of Molecular Properties. *Journal of Physical Chemistry Letters*, **2017**, 8, 1351-1359	6.4	44
20	Machine Learning, Quantum Chemistry, and Chemical Space. *Reviews in Computational Chemistry*, **2017**, 225-256		41
19	Fast and accurate predictions of covalent bonds in chemical space. *Journal of Chemical Physics*, **2016**, 144, 174110	3.9	33
18	Generalized Density-Functional Tight-Binding Repulsive Potentials from Unsupervised Machine Learning. *Journal of Chemical Theory and Computation*, **2018**, 14, 2341-2352	6.4	32
17	Semi-quartic force fields retrieved from multi-mode expansions: Accuracy, scaling behavior, and approximations. *Journal of Chemical Physics*, **2015**, 142, 154118	3.9	26
16	The DFT+U method in the linear combination of Gaussian-type orbitals framework: Role of 4f orbitals in the bonding of LuF3. *Chemical Physics Letters*, **2009**, 468, 158-161	2.5	18
15	Control and analysis of single-determinant electron dynamics. *Physical Review A*, **2012**, 85,	2.6	16
14	The chemical space of B, N-substituted polycyclic aromatic hydrocarbons: Combinatorial enumeration and high-throughput first-principles modeling. *Journal of Chemical Physics*, **2019**, 150, 114106	3.9	11
13	Electron dynamics across molecular wires: A time-dependent configuration interaction study. *Chemical Physics*, **2013**, 420, 44-49	2.3	11
12	Charge transfer dynamics from adsorbates to surfaces with single active electron and configuration interaction based approaches. *Chemical Physics*, **2015**, 446, 24-29	2.3	7

11	Torsional Potentials of Glyoxal, Oxalyl Halides, and Their Thiocarbonyl Derivatives: Challenges for Popular Density Functional Approximations. *Journal of Chemical Theory and Computation*, **2018**, 14, 4806-4817	6.4	7
10	Revving up 13C NMR shielding predictions across chemical space: benchmarks for atoms-in-molecules kernel machine learning with new data for 134 kilo molecules. *Machine Learning: Science and Technology*, **2021**, 2, 035010	5.1	6
9	Quantum-chemistry-aided identification, synthesis and experimental validation of model systems for conformationally controlled reaction studies: separation of the conformers of 2,3-dibromobuta-1,3-diene in the gas phase. *Physical Chemistry Chemical Physics*, **2020**, 22, 13431-13439	3.6	5
8	Critical benchmarking of popular composite thermochemistry models and density functional approximations on a probabilistically pruned benchmark dataset of formation enthalpies. *Journal of Chemical Physics*, **2021**, 154, 044113	3.9	5
7	Machine learning modeling of Wigner intracule functionals for two electrons in one-dimension. *Journal of Chemical Physics*, **2019**, 150, 144114	3.9	3
6	Charge-transfer selectivity and quantum interference in real-time electron dynamics: Gaining insights from time-dependent configuration interaction simulations. *Journal of Chemical Physics*, **2020**, 152, 194111	3.9	3
5	High-throughput design of Peierls and charge density wave phases in Q1D organometallic materials. *Journal of Chemical Physics*, **2021**, 154, 061102	3.9	2
4	Data-driven modeling of S -yS excitation energy in the BODIPY chemical space: High-throughput computation, quantum machine learning, and inverse design.. *Journal of Chemical Physics*, **2021**, 155, 244102	3.9	2
3	Machine learning modeling of materials with a group-subgroup structure. *Machine Learning: Science and Technology*, **2021**, 2, 035035	5.1	1
2	Exact separation of radial and angular correlation energies in two-electron atoms. *Chemical Physics Letters*, **2019**, 720, 93-96	2.5	1
1	Troubleshooting unstable molecules in chemical space. *Chemical Science*, **2021**, 12, 5566-5573	9.4	1