

# Andrea Grisafi

## List of Publications by Year in Descending Order

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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.

15  
papers

590  
citations

10  
h-index

15  
g-index

15  
ext. papers

871  
ext. citations

10  
avg, IF

4.77  
L-index

#	Paper	IF	Citations
15	Learning Electron Densities in the Condensed Phase. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 7203-7214	6.4	2
14	Physics-Inspired Structural Representations for Molecules and Materials. <i>Chemical Reviews</i> , <b>2021</b> , 121, 9759-9815	68.1	50
13	Learning (from) the Electron Density: Transferability, Conformational and Chemical Diversity. <i>Chimia</i> , <b>2020</b> , 74, 232-236	1.3	6
12	Multi-scale approach for the prediction of atomic scale properties. <i>Chemical Science</i> , <b>2020</b> , 12, 2078-2090	9.4	15
11	Electron density learning of non-covalent systems. <i>Chemical Science</i> , <b>2019</b> , 10, 9424-9432	9.4	55
10	Quantum mechanical static dipole polarizabilities in the QM7b and AlphaML showcase databases. <i>Scientific Data</i> , <b>2019</b> , 6, 152	8.2	13
9	Accurate molecular polarizabilities with coupled cluster theory and machine learning. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2019</b> , 116, 3401-3406	11.5	71
8	Using Gaussian process regression to simulate the vibrational Raman spectra of molecular crystals. <i>New Journal of Physics</i> , <b>2019</b> , 21, 105001	2.9	30
7	Incorporating long-range physics in atomic-scale machine learning. <i>Journal of Chemical Physics</i> , <b>2019</b> , 151, 204105	3.9	58
6	Atomic-Scale Representation and Statistical Learning of Tensorial Properties. <i>ACS Symposium Series</i> , <b>2019</b> , 1-21	0.4	9
5	Transferable Machine-Learning Model of the Electron Density. <i>ACS Central Science</i> , <b>2019</b> , 5, 57-64	16.8	114
4	Symmetry-Adapted Machine Learning for Tensorial Properties of Atomistic Systems. <i>Physical Review Letters</i> , <b>2018</b> , 120, 036002	7.4	136
3	Solvent fluctuations and nuclear quantum effects modulate the molecular hyperpolarizability of water. <i>Physical Review B</i> , <b>2017</b> , 96,	3.3	22
2	Localized Polycentric Orbital Basis Set for Quantum Monte Carlo Calculations Derived from the Decomposition of Kohn-Sham Optimized Orbitals. <i>Computation</i> , <b>2016</b> , 4, 10	2.2	2
1	Roadmap on Machine Learning in Electronic Structure. <i>Electronic Structure</i> ,	2.6	7