Andrea Grisafi

List of Publications by Year
in descending order

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		759233	996975
15	1,187	12	15
papers	citations	h-index	g-index

15	15	15	933
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Roadmap on Machine learning in electronic structure. Electronic Structure, 2022, 4, 023004.	2.8	69
2	Multi-scale approach for the prediction of atomic scale properties. Chemical Science, 2021, 12, 2078-2090.	7.4	35
3	Physics-Inspired Structural Representations for Molecules and Materials. Chemical Reviews, 2021, 121, 9759-9815.	47.7	247
4	Learning Electron Densities in the Condensed Phase. Journal of Chemical Theory and Computation, 2021, 17, 7203-7214.	5.3	24
5	Learning (from) the Electron Density: Transferability, Conformational and Chemical Diversity. Chimia, 2020, 74, 232-236.	0.6	9
6	Using Gaussian process regression to simulate the vibrational Raman spectra of molecular crystals. New Journal of Physics, 2019, 21, 105001.	2.9	44
7	Electron density learning of non-covalent systems. Chemical Science, 2019, 10, 9424-9432.	7.4	92
8	Quantum mechanical static dipole polarizabilities in the QM7b and AlphaML showcase databases. Scientific Data, 2019, 6, 152.	5.3	20
9	Accurate molecular polarizabilities with coupled cluster theory and machine learning. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 3401-3406.	7.1	126
10	Incorporating long-range physics in atomic-scale machine learning. Journal of Chemical Physics, 2019, 151, 204105.	3.0	114
11	Atomic-Scale Representation and Statistical Learning of Tensorial Properties. ACS Symposium Series, 2019, , 1-21.	0.5	12
12	Transferable Machine-Learning Model of the Electron Density. ACS Central Science, 2019, 5, 57-64.	11.3	178
13	Symmetry-Adapted Machine Learning for Tensorial Properties of Atomistic Systems. Physical Review Letters, 2018, 120, 036002.	7.8	186
14	Solvent fluctuations and nuclear quantum effects modulate the molecular hyperpolarizability of water. Physical Review B, 2017, 96, .	3.2	28
15	Localized Polycentric Orbital Basis Set for Quantum Monte Carlo Calculations Derived from the Decomposition of Kohn-Sham Optimized Orbitals. Computation, 2016, 4, 10.	2.0	3