Andrea Grisafi

List of Publications by Year
in descending order

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Version: 2024-02-01

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