# Andrea Grisafi

## List of Publications by Citations



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