

# Michael J Willatt

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/3791928/publications.pdf>

Version: 2024-02-01

12  
papers

729  
citations

840585

11  
h-index

1199470

12  
g-index

12  
all docs

12  
docs citations

12  
times ranked

679  
citing authors

#	ARTICLE	IF	CITATIONS
1	Atom-density representations for machine learning. <i>Journal of Chemical Physics</i> , 2019, 150, 154110.	1.2	120
2	Incompleteness of Atomic Structure Representations. <i>Physical Review Letters</i> , 2020, 125, 166001.	2.9	103
3	Fast and Accurate Uncertainty Estimation in Chemical Machine Learning. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 906-915.	2.3	102
4	Communication: Relation of centroid molecular dynamics and ring-polymer molecular dynamics to exact quantum dynamics. <i>Journal of Chemical Physics</i> , 2015, 142, 191101.	1.2	90
5	Boltzmann-conserving classical dynamics in quantum time-correlation functions: Matsubara dynamics. <i>Journal of Chemical Physics</i> , 2015, 142, 134103.	1.2	89
6	Feature optimization for atomistic machine learning yields a data-driven construction of the periodic table of the elements. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 29661-29668.	1.3	88
7	Path-integral dynamics of water using curvilinear centroids. <i>Journal of Chemical Physics</i> , 2019, 151, .	1.2	36
8	Efficient implementation of atom-density representations. <i>Journal of Chemical Physics</i> , 2021, 154, 114109.	1.2	32
9	Approximating Matsubara dynamics using the planetary model: Tests on liquid water and ice. <i>Journal of Chemical Physics</i> , 2018, 148, 102336.	1.2	27
10	Equivariant representations for molecular Hamiltonians and $\langle i \rangle_N \langle i \rangle$ -center atomic-scale properties. <i>Journal of Chemical Physics</i> , 2022, 156, 014115.	1.2	26
11	Atomic-Scale Representation and Statistical Learning of Tensorial Properties. <i>ACS Symposium Series</i> , 2019, , 1-21.	0.5	12
12	Machine-Learning of Atomic-Scale Properties Based on Physical Principles. <i>Lecture Notes in Physics</i> , 2020, , 99-127.	0.3	4