

# Jonathan Vandermause

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/267499/publications.pdf>

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1478505

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times ranked

433  
citing authors

#	ARTICLE	IF	CITATIONS
1	On-the-fly active learning of interpretable Bayesian force fields for atomistic rare events. Npj Computational Materials, 2020, 6, .	8.7	199
2	Accurate and scalable graph neural network force field and molecular dynamics with direct force architecture. Npj Computational Materials, 2021, 7, .	8.7	63
3	Evolution of Metastable Structures at Bimetallic Surfaces from Microscopy and Machine-Learning Molecular Dynamics. Journal of the American Chemical Society, 2020, 142, 15907-15916.	13.7	47
4	Bayesian force fields from active learning for simulation of inter-dimensional transformation of stanene. Npj Computational Materials, 2021, 7, .	8.7	33
5	A fast neural network approach for direct covariant forces prediction in complex multi-element extended systems. Nature Machine Intelligence, 2019, 1, 471-479.	16.0	32
6	Multitask Machine Learning of Collective Variables for Enhanced Sampling of Rare Events. Journal of Chemical Theory and Computation, 2022, 18, 2341-2353.	5.3	25