

# Ferenc Karsai

## List of Publications by Year in descending order

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572  
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#	ARTICLE	IF	CITATIONS
1	Phase Transitions of Hybrid Perovskites Simulated by Machine-Learning Force Fields Trained on the Fly with Bayesian Inference. Physical Review Letters, 2019, 122, 225701.	7.8	250
2	On-the-fly machine learning force field generation: Application to melting points. Physical Review B, 2019, 100, .	3.2	233
3	On-the-Fly Active Learning of Interatomic Potentials for Large-Scale Atomistic Simulations. Journal of Physical Chemistry Letters, 2020, 11, 6946-6955.	4.6	100
4	Descriptors representing two- and three-body atomic distributions and their effects on the accuracy of machine-learned inter-atomic potentials. Journal of Chemical Physics, 2020, 152, 234102.	3.0	71
5	Thermal transport and phase transitions of zirconia by on-the-fly machine-learned interatomic potentials. Npj Computational Materials, 2021, 7, .	8.7	57
6	Making free-energy calculations routine: Combining first principles with machine learning. Physical Review B, 2020, 101, .	3.2	35
7	$\pm \hat{I}^2$ phase transition of zirconium predicted by on-the-fly machine-learned force field. Physical Review Materials, 2021, 5, .	2.4	21
8	Phase transitions of zirconia: Machine-learned force fields beyond density functional theory. Physical Review B, 2022, 105, .	3.2	21
9	First-principles hydration free energies of oxygenated species at water–platinum interfaces. Journal of Chemical Physics, 2021, 154, 094107.	3.0	11