# Ferenc Karsai

## List of Publications by Year
in descending order

| | | |
|---|---|---|
| **9**<br>papers | **799**<br>citations | 1039406<br>**9**<br>h-index | 1473754<br>**9**<br>g-index |
| **9**<br>all docs | **9**<br>docs citations | **9**<br>times ranked | **572**<br>citing authors |

| # | Article | IF | Citations |
|---|---------|-----|-----------|
| 1 | Phase transitions of zirconia: Machine-learned force fields beyond density functional theory. Physical Review B, 2022, 105, . | 1.1 | 21 |
| 2 | First-principles hydration free energies of oxygenated species at waterâ€"platinum interfaces. Journal of Chemical Physics, 2021, 154, 094107. | 1.2 | 11 |
| 3 | <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>Î±</mml:mi><mml:mtext>â^’</mml:mtext><mml:mi>Î²</mml:mi></mml phase transition of zirconium predicted by on-the-fly machine-learned force field. Physical Review Materials, 2021, 5, . | 0.9 | 21 |
| 4 | Thermal transport and phase transitions of zirconia by on-the-fly machine-learned interatomic potentials. Npj Computational Materials, 2021, 7, . | 3.5 | 57 |
| 5 | On-the-Fly Active Learning of Interatomic Potentials for Large-Scale Atomistic Simulations. Journal of Physical Chemistry Letters, 2020, 11, 6946-6955. | 2.1 | 100 |
| 6 | 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. | 1.2 | 71 |
| 7 | Making free-energy calculations routine: Combining first principles with machine learning. Physical Review B, 2020, 101, . | 1.1 | 35 |
| 8 | On-the-fly machine learning force field generation: Application to melting points. Physical Review B, 2019, 100, . | 1.1 | 233 |
| 9 | Phase Transitions of Hybrid Perovskites Simulated by Machine-Learning Force Fields Trained on the Fly with Bayesian Inference. Physical Review Letters, 2019, 122, 225701. | 2.9 | 250 |