# Michael J Willatt

List of Publications by Year
in descending order



| 12 | 729 | 840585 11 | 1199470 12 |
|---|---|---|---|
| papers | citations | h-index | g-index |

| 12 | 12 | 12 | 679 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

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