



Keiran Thompson

Research Scientist

Chemistry

Bio

ACADEMIC APPOINTMENTS

- Phys Sci Res Assoc, Chemistry

Publications

PUBLICATIONS

- **ChemPix: automated recognition of hand-drawn hydrocarbon structures using deep learning** *CHEMICAL SCIENCE*
Weir, H., Thompson, K., Woodward, A., Choi, B., Braun, A., Martinez, T. J.
2021
- **The non-adiabatic nanoreactor: towards the automated discovery of photochemistry** *CHEMICAL SCIENCE*
Pieri, E., Lahana, D., Chang, A. M., Aldaz, C. R., Thompson, K. C., Martinez, T. J.
2021
- **TeraChem Cloud: A High-Performance Computing Service for Scalable Distributed GPU-Accelerated Electronic Structure Calculations.** *Journal of chemical information and modeling*
Seritan, S. n., Thompson, K. n., Martínez, T. J.
2020
- **Construction of reaction networks using the ab initio nanoreaction coupled to a kinetic model**
Meisner, J., Zhu, X., Thompson, K., Hirai, H., Martinez, T.
AMER CHEMICAL SOC.2019
- **Methane combustion studied using the ab initio nanoreactor approach combined with kinetic modeling**
Meisner, J., Zhu, X., Hirai, H., Thompson, K., Martinez, T.
AMER CHEMICAL SOC.2019
- **Geodesic interpolation for reaction pathways** *JOURNAL OF CHEMICAL PHYSICS*
Zhu, X., Thompson, K. C., Martinez, T. J.
2019; 150 (16)
- **Thinking inside boxes: Modularizing electronic structure and ab initio molecular dynamics**
Seritan, S., Thompson, K., Fales, S., Song, C., Parrish, R., Hohenstein, E., Martinez, T.
AMER CHEMICAL SOC.2019
- **Large-Scale Functional Group Symmetry-Adapted Perturbation Theory on Graphical Processing Units** *JOURNAL OF CHEMICAL THEORY AND COMPUTATION*
Parrish, R. M., Thompson, K. C., Martinez, T. J.
2018; 14 (3): 1737–53