

Alexander Michael Chang

Ph.D. Student in Chemistry, admitted Autumn 2019

Publications

PUBLICATIONS

- **Efficient Acceleration of Reaction Discovery in the Ab Initio Nanoreactor: Phenyl Radical Oxidation Chemistry.** *The journal of physical chemistry. A*
Chang, A. M., Meisner, J., Xu, R., Martínez, T. J.
2023
- **First principles reaction discovery: from the Schrodinger equation to experimental prediction for methane pyrolysis.** *Chemical science*
Xu, R., Meisner, J., Chang, A. M., Thompson, K. C., Martínez, T. J.
2023; 14 (27): 7447-7464
- **First principles reaction discovery: from the Schrodinger equation to experimental prediction for methane pyrolysis** *CHEMICAL SCIENCE*
Xu, R., Meisner, J., Chang, A. M., Thompson, K. C., Martínez, T. J.
2023
- **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., Martínez, T. J.
2021; 12 (21): 7294-7307
- **Hammett neural networks: prediction of frontier orbital energies of tungsten-benzylidyne photoredox complexes** *CHEMICAL SCIENCE*
Chang, A. M., Freeze, J. G., Batista, V. S.
2019; 10 (28): 6844-54
- **Inverse Design of a Catalyst for Aqueous CO/CO₂ Conversion Informed by the Ni-II-Iminothiolate Complex** *INORGANIC CHEMISTRY*
Chang, A. M., Rudshteyn, B., Warnke, I., Batista, V. S.
2018; 57 (24): 15474-80