Stefan Seritan
Ph.D. Student in Chemistry, admitted Autumn 2015

Publications

PUBLICATIONS

• 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 Electron Correlation Calculations: Rank-Reduced Full Configuration Interaction. Journal of chemical theory and computation
  Fales, B. S., Seritan, S., Settje, N. F., Levine, B. G., Koch, H., Martínez, T. J.
  2018

• Viewpoints on the 2017 American Conference on Theoretical Chemistry JOURNAL OF PHYSICAL CHEMISTRY A
  Goldsmith, Z. K., Provazza, J., Seritan, S.
  2017; 121 (41): 7807–12

• Rate-Enhancing Roles of Water Molecules in Methyliqtrioxorhenium-Catalyzed Olefin Epoxidation by Hydrogen Peroxide JOURNAL OF THE AMERICAN CHEMICAL SOCIETY
  2015; 137 (30): 9604–16

• A design equation for low dosage additives that accelerate nucleation FARADAY DISCUSSIONS
  Poon, G. G., Seritan, S., Peters, B.
  2015; 179: 329–41