Abstract Submitted
for the 4CS20 Meeting of
The American Physical Society

Methods in Computational Enzyme Design AUSTIN JARRETT, Brigham Young University — Enzyme engineering is a powerful field that makes use of physical, chemical, biological, and computational principles to develop novel catalysts for desired chemical products. Traditional methods of enzyme engineering require many rounds of mutation and screening for desired properties. In recent years, computational enzyme design has emerged as an attractive alternative to traditional techniques to reduce time and cost with increased ability to explore the vast sequence space. A wide variety of computational tools and methods have been developed in to aid in computational enzyme design. Over 80 published studies in the field of enzyme engineering from the past five years have been studied and categorized to evaluate differences in computational approaches and strengths of each one. This search has provided valuable insight regarding areas requiring improvement in this field and possible future applications of these tools.

Austin Jarrett
Brigham Young University

Date submitted: 29 Sep 2020 Electronic form version 1.4