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Abstract for an Invited Paper
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Application, Assessment, and Development of Molecular Design Methods[1]

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Over millions of years, proteins have evolved to fulfill a plethora of life sustaining tasks. Even under physiological constraints, such as pH, temperature, and intracellular densities, they have adapted to accomplish specific tasks with high efficiency. Additionally, everything that defines a protein is encoded in its primary amino acid sequence, from its folded structure to its dynamical ensemble of states and the chemical universe that it can interact with. For decades humanity has sought to harness the power of proteins for new and important processes. While we have gained many important insights along the way, mankind still falls short of fully reproducing nature's remarkable ability to build custom nano machines. The de novo design of catalysts that mimic the affinity and specificity of natural enzymes remains one of the Holy Grails of chemistry. Despite decades of concerted effort, we are still unable to design catalysts as efficient as enzymes. However, imagine what we could accomplish if we had the skills to create proteins with high catalytic rates for crucial reactions, such as photosynthesis, plastic degradation, or nitrogen fixation! The Della Corte lab at BYU operates at the intersection of physics, biology, chemistry, chemical engineering, and computer science. It has the goal to learn the governing principles of molecular design and to apply these to solve world changing problems. This presentation will provide an overview of recent and current activities that leverage AI and physics based simulations to apply, assess, and develop molecular design methods at Della Corte lab at BYU.

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