The advent of innovative molecular modeling algorithms, optimization strategies, and machine learning techniques is ushering a new era of engineering in which computational tools are routinely used to probe, design, and interrogate complex fluids, materials, and even functional materials systems. In this presentation, I will illustrate some of these ideas in the context of several examples taken from chemical engineering, physics, biology, and materials science and engineering. These examples can be categorized into three areas. In the first, advanced models and procedures are used to extract information from simultaneous, high-information-content experiments. In the second, machine learning techniques are used to develop advanced molecular models of fluids or materials. In the third, machine learning and advanced optimization strategies are used to identify design rules and to create new materials. By discussing one example from each of these categories, this presentation will seek to provide a broad perspective on how artificial intelligence might be used to enhance thermophysical property research.