Machine learning approaches for modeling metal and alloy surfaces

John Kitchin†
Carnegie Mellon University
(jkitchin@andrew.cmu.edu†)

Machine learning offers a path forward to build models that are not necessarily based on physics, but which more accurately predict outputs. We are interested in building models that allow us to perform molecular simulations that require many (hundreds of thousands) of calculations. These are not practical with quantum chemical calculations, which are too expensive to run at this scale. Existing molecular force fields are efficient enough for this, however, they lack the accuracy required to obtain meaningful results. I will present how we are using machine learning in conjunction with quantum chemical calculations to develop efficient models that can be used to simulate effects such as segregation, diffusion, etc., which can only be probed using simulation methods such as Monte Carlo and molecular dynamics. This approach is not fool-proof though, and we will show examples that worked well, and what we have learned from examples that did not work as well.