Physics based machine learning for materials and compound space

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Many of the most relevant observables of matter depend explicitly on atomistic and electronic structure, rendering physics based approaches to chemistry and materials necessary. Unfortunately, due to the combinatorial scaling of the number of chemicals and potential reaction settings, gaining a holistic and rigorous understanding through exhaustive quantum and statistical mechanics based sampling is prohibitive --- even when using high-performance computers. Accounting for explicit and implicit dependencies and correlations, however, will not only deepen our fundamental understanding but also benefit exploration campaigns (computational and experimental). I will discuss recently gained insights from my labs elucidating such relationships thanks to supervised machine learning.