Leveraging big data and chemical reaction networks to explore and explain electrochemistry

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From storing renewable energy to improving the efficiency of organic synthesis, electrochemistry is well poised to drive the global technological transformation towards sustainability. However, the design of new battery materials and electrocatalysts is hampered by slow and labor-intensive trial and error. The rational design of electrochemical systems will only be possible when the underlying reaction and transport mechanisms can be understood and predicted from first principles. In this talk, I will discuss how theory can be used to explain reactive phenomena and move towards rational design, even in complex domains. I will describe my recent work, which aims to predict the properties of electrochemical processes by combining high-throughput quantum chemistry, big data, and chemical reaction networks (CRNs). Using electrolyte decomposition and solid electrolyte interphase formation in lithium-ion batteries as an exemplar system, I will demonstrate how data-driven CRNs can be leveraged to identify key species (e.g. reaction products), predict formation mechanisms, and even elucidate reactive competition between different species and reaction pathways. To conclude, I will present a vision of applying the theoretical tools of reaction exploration to not only improve our knowledge of existing technologies, but also to accelerate the development of unexplored chemical systems.