Exascale computing methods for the design of new battery materials and catalysts

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Abstract: Theoretical chemists and material scientists have spent decades developing computational methods and software for understanding how materials function, such as for battery materials and catalysts. In recent years, due to constantly improving methods and faster computers, we are also able to tackle the inverse problem of designing new materials which have a better functionality, such as higher efficiencies for catalysts, as well as improved voltage and capacity for battery materials. Looking to the future, we need to adapt our computational methods and software for massively parallel exascale computing resources. Most of our computational methods, including the ubiquitous density functional theory for approximating electronic structure, scale poorly with the number of compute cores available. Recent methods borrowed from computer science in the area of machine learning are making is possible to approximate density functional theory calculations when there is sufficient data available for training. What is needed, and what is being proposed here, is to develop algorithms that can take advantage of exascale computational heterogeneous resources to accelerate modeling of materials at the atomic scale and also facilitate the design of new materials for energy applications.