The tricky question of Material Design in Computational Material Science

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Materials Science is increasingly appealing to computational models and methods to handle the complexity of materials shape and reactivity in various technological applications. Material Design has emerged as a new field in which the ultimate goal is to conceive, in silico, new materials with improved targeted properties. In the specific area of energy storage, the Material Project Initiative has initiated massive algorithmic developments and informatics strategies. This has led to unquestionable successes of data-driven analyses in very different domains. Using material properties data and advanced computer models, the behavior of new materials can then be predicted, so as to avoid lengthy cycles of build and test. These simulations cover a wide range of operating environments and length and time scales. However, when the targeted property is a response function of the materials, the question of which data are relevant to use in machine learning algorithm is more ambiguous. I will review these questions in the case of materials for energy storage applications and present the new challenge of data standardization for the very complex issue of interfaces in electrochemical devices.