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Materials Design on Three Fronts: Fundamental Theory, Automation, and Artificial Intelligence

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Abstract: The design of new materials with specific properties is at the core of our technological progress. I will present our ongoing efforts in this field, spanning over three connected topical areas: (i) fundamental theory development for improved exchange-correlation functionals in density-functional theory (DFT); (ii) progress on software for high-level automation of materials property calculations and its application to materials design; and (iii) the adoption of methods from big data and machine learning for prediction, data mining, and visual exploration in ways that greatly expand the reach and scope of traditional methods. On the topic of fundamental theory development, I discuss a recent semi-local functional for DFT that better mimics the states (and thus band structure) of higher order methods. In automation, I highlight a few features in the software toolkit we use which are distinct from other efforts (primarily AiiDA and the materials project software stack) and show recent examples of its application for high-throughput materials design of piezoelectrics. In big data and machine learning, I discuss a machine-learning model demonstrated to, at the cost of 10k DFT calculations, predict 2M DFT-quality formation energies of substitutions into the elpasolite crystal structure, which facilitates the identification of 128 new stable elpasolites.