Computational discovery and design of perovskites

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During the past decade halide peroskites have revolutionized research on solar photovoltaics. With a solar-to-electricity power conversion efficiency above 25%, halide perovskites are the first solution-processable technology to rival silicon photovoltaics. In this talk I will discuss how computational materials research and atomic-scale quantum simulations can contribute to this vast and exciting field. I will illustrate successful strategies for the computational design of new perovskites and double perovskites using combinatorial chemistry and geometric descriptors. I will show how these approaches, when integrated with experimental synthesis and characterization, can deliver new materials with high potential in photovoltaics and lighting technology. Finally, I will argue that only a small subset of all possible perovskites is currently known, and much work is still needed to discover new materials of this family and to explore their technological uses. If time allows, I will present some data on new nitride perovskites that we recently predicted but have not yet been synthesized.