Computer Simulations for Better Solar Cells

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In this talk, I will present some of our recent work dedicated to simulations of lead halide perovskite based solar cells that are aimed at gaining an atomistic understanding of the fundamental mechanisms that govern the function and stability of such devices. This, work is based on many of Michele Parrinello's seminal methodological contributions ranging from Parrinello-Rahman flexible cell molecular dynamics (MD), to Car-Parrinello first-principles MD, enhanced sampling methods and machine learning potentials.