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Force field development from first principles for materials design MARIA CHAN, ALPER KINACI, BADRI NARAYANAN, FATIH SEN, STEPHEN GRAY, MICHAEL DAVIS, SUBRAMANIAN SANKARANARYANAN, Argonne National Laboratory — The ability to perform accurate calculations efficiently is crucial for computational materials design. In this talk, we will discuss a stream-lined approach to force field development using first principles density functional theory training data and machine learning algorithms. We will also discuss the validation of this approach on precious metal nanoparticles.

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