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ASE, GPAW, CMR, and that kind of tools

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ABSTRACT

During the last decades we have developed several, mostly Python-based, tools for setting up, controlling/steering, storing, analyzing, and sharing simulations at the atomic and electronic scale. In particular, we have developed the Atomic Simulation Environment which has become a fairly widely used scripting tool for setting up and controlling simulations with either an interatomic potential code or an electronic structure code as “backends” for the force and energy calculations. More recently, we have developed a real-space density-functional-theory and many-body-perturbation-theory code, GPAW, and most recently the Computational Materials Repository for storing, sharing, and retrieving atomic-scale data. In the discussion, I shall present some of the experiences we have gained through these developments and show some examples of their recent to the problem of finding new materials for efficient solar energy conversion into electricity or fuels.