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Large scale *ab initio* ground and excited state calculations using the OpenAtom software

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OpenAtom is a massively parallel plane wave pseudopotential software exhibiting high quality scaling to large numbers of processors by taking advantage of the Charm++ parallel framework (http://charm.cs.uiuc.edu/OpenAtom). At present, the software can perform ground-state molecular dynamics (MD) simulations (Car-Parrinello or Born-Oppenheimer) together with k-points, spin, path integral molecular dynamics for quantum nuclear effects, and parallel tempering for exploration of complex phase spaces. Some of these MD capabilities will be highlighted using our ongoing studies on large metal organic framework (MOF) materials of scientific and potential technological interest for hydrogen storage. Separately, we are in the process of adding electronic excitation capabilities to OpenAtom within the GW approximation to enable more accurate descriptions of quasiparticle energy band structures. Progress on the development and large-scale parallelization of the GW software implementation will be presented.

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