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New implementations for large scale DFT and GW calculations with numeric atom-centered orbital basis functions on many-core architectures[1] ALVARO VAZQUEZ MAYAGOITIA, Argonne Leadership Computing Facility — Advances in recent implementations in FHI-aims code (https://aimsclub.fhi-berlin.mpg.de/) to exploit many-core architectures with multi-level parallelism, by combining Message Passing Interface programing and OpenMP threads, are presented. FHI-aims which is an all-electron code and uses numeric atom-centered orbital basis was modified to effectively use thousands of cores and compute large scale electronic structure calculations of solids and clusters. This advances enabled high-throughput and data analytic driven approaches for material discovery. Extensive benchmark results in many-core petascale computers using DFT calculations, with dispersion corrected hybrid functionals, and GW approaches in molecular crystals are also presented.

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Alvaro Vazquez Mayagoitia
Argonne Leadership Computing Facility

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