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STRUCTURE PROPERTY RELATIONSHIPS IN ORGANIC SOLAR CELLS MATERIALS

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HPC content

I use the HPc mainly for optimizing structures that are between 60 to 500 atoms using ab_initio kind of calculations. The application code used is NWchem_6.6. Normally the calculations are done using 240 cores and a total memory of 10000 Mb. Since Nwchem is made to run on multiple nodes the MPI scales very well upto 6 nodes using all cores.

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