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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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