GaN Jobs

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1 DFT

1.1 b3pw91

1.1.1 szv

- 111 Converged, but not plotted with
  WARN: 2.03 error found in overlap integrals. cell.precision or cell.rcut
  can be adjusted to improve accuracy
  and
  kmf.get_bands()
  updated pyscf
  5 running from scatch 11-14
  6 running from scratch with rcut adjusted 11-14
  plotted

- 222 same as 111
  now going to 7 running from scratch with rcut adjusted 11-14
  plotted

- 333 not converged and give more time and cores
  4 running from scratch 11-14
  making 5 with rcut adjusted 11-14
  still running

1.1.2   dzvp

- 111
  Converged and plotted

- 222
  Converged and plotted

- 333
  idk trying to restart but not going
  game plan is two start from scratch with a longer time and more coarse
  6_scratch ready to roll 11-14
  need to just plot it
  plotted

1.2   pbe

1.2.1   szv

- 111
  running first iterations for touting
  plotted

- 222
  running first iterations for touting
  plotted

- 333
  running first iterations for touting
  plotted

1.2.2   dzvp

- 111
  running first iterations for touting
  plotted

- 222
  running first iterations for touting
  plotted

- 333
  running first iterations for touting
  plotted