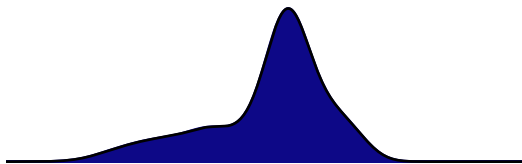


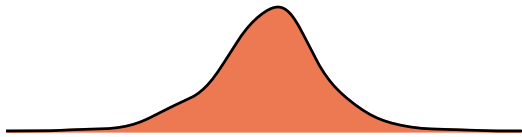
Empirical



Physical (MM)



Physical (QM)



-5                      0                      5

$\Delta \log P$  error (calc - exp)