Notes on convergence tests for datasets

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It is our experience that PAW datasets can behave somewhat differently within different codes. For example, in some of our studies, the calculations converged very well for a kinetic energy cutoff for representing the wavefunctions of ecut=25 H (50 Ry) using ABINIT, while for QUANTUM ESPRESSO, ecutwfc=60-70 Ry is needed. As an example, the figure below shows a plot of the calculated energy differences of relaxed structures of $Na_4P_2S_6$ as a function of the kinetic energy cutoffs for the two codes. Happily, the two results converge to essentially the same energy. However the ABINIT results are converged at a smaller cutoff value than the QUANTUM ESPRESSO results for this case.

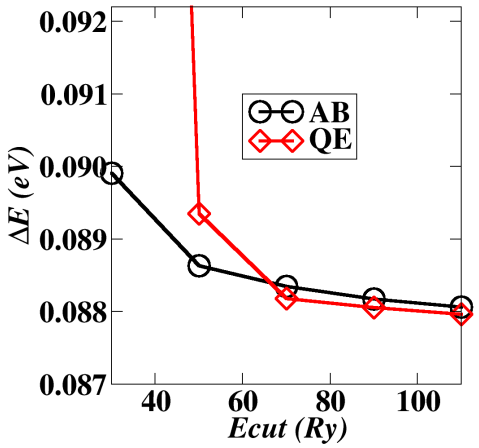


**Fig.** Plot of the energy difference between optimized structures of $Na_4P_2S_6$ in the hexagonal $P\bar{3}1m$ (#162 in the International Table of Crystallography) relative to the centered monoclinic structure $C2/m$ (#12) as a function of the kinetic energy cutoff energy used in the calculation. Results are given in units of eV/Formula Unit and calculations were performed with the ABINIT (AB) and the QUANTUM ESPRESSO (QE) codes using the PBESOL functional.