Calculations of Phonon Properties in Oxides, and of Dielectric Functions in Halides

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I tried the phonon calculations for oxides by using "phonopy" to obtain its dispersion and density of states. Supercells with displacements are needed to be created for the calculations of phonon dispersion and/or their density of states. Number of the created configurations is dependent on the symmetry of the relevant crystal (see, for example, Table 1). In other words, a number of *ab-initio* supercell calculations have to be executed to obtain force on atoms, though they are binary materials (N_{atom}=2). Due to the abovementioned situations, I have not completed the tasks. Despite this fact, I have already successfully created a force constants file for one of these oxides. The related postprocess will be performed sequentially, because this package can be executed even under Linux-based personal computers.

material	symmetry	configuration	N_{typ}	N_{atom}
A	Pnma	40	40	2
B	Pnma	40	40	2
C	Pnma	60	40	2

I also tried dielectric function calculations for halide-based mixed crystals. Because the dielectric function cannot be directly converted from the spectral distribution of the density of states, so I tried to calculate them by using "RESPACK". I was able to finally master how to convert the self-consistent field calculation results from "Quantum ESPRESSO" to "RESPACK" formats by communicating with the staffs. The validity and comparison with our experimental data of the partially obtained results are being checked currently.

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References

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[2] L. Chaput, A. Togo, I. Tanaka, and G. Hug, Phys. Rev. B, **84** (2011) 094302.