Reproducibility in response calculations of solids

G. Petretto[1], M. Giantomassi[1], and G.-M. Rignanese[1]

[1] Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Belgium

Recently efforts have been devoted to evaluating the response properties (elastic tensors, phonon band structures, dielectric tensors, piezoelectric tensors) for a large number of compounds [1-8] which have been made accessible online [9-11]. These results have been obtained with different codes (VASP, QUANTUM ESPRESSO, and ABINIT) and different methods (finite differences and density functional perturbation theory). Similar to the effort that was undertaken for assessing the reproducibility of density functional theory calculations [8], there is a need to evaluate the reproducibility of response calculations of solids.

In this talk, we will share some ideas on this topic. We will also discuss the possible standardization that may result from the effort to be undertaken.

References

[1] A. Togo and I. Tanaka, Scr. Mater. **108**, 1 (2015)

[2] M. de Jong *et al.*, Sci. Data **2**, 150009 (2015)

[3] M. de Jong *et al.*, Sci. Data **2**, 150053 (2015)

[4] I. Petousis *et al.*, Phys. Rev. B **93**, 115151 (2016)

[5] I. Petousis *et al.*, Sci. Data **4**, 160134 (2017)

[6] N. Mounet *et al.*, Nat. Nanotechnol. **13**, 246 (2018)

[7] G. Petretto *et al.*, Comp. Mater. Sci. **144**, 331-337 (2018)

[8] G. Petretto *et al.*, Sci. Data **5**, 180065 (2018)

[9] http://phonondb.mtl.kyoto-u.ac.jp

[10] http://www.materialscloud.org

[11] http://www.materialsproject.org

[12] K. Lejaeghere *et al.*, Science **351**, aad3000 (2016)