

# The Delta project: current status and future directions

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*Do different density-functional theory (DFT) codes yield the same results?* Even when the used exchange-correlation functional is the same, the answer to this question is not straightforward. A collaboration, encompassing more than 40 institutes and about 70 individual researchers, was therefore set up to investigate the precision of current DFT codes and (pseudo)potential libraries in terms of the  $\Delta$  gauge [1]. The outcome of this project is now available [2,3] and is reassuring: recent implementations of the PBE functional – be it in all-electron codes, PAW packages or pseudopotential programmes – yield energy versus volume curves that vary only as much as high-quality experimental values differ from each other.

A major follow-up question entails the transferability of these first conclusions. Several extension of the Delta project are now being set up, benchmarking different functionals, materials and properties. In addition, the original Delta benchmark is publicly available and is still being added to. Such a database can serve to calibrate new emerging DFT codes and potentials, and as a quality indicator towards mainstream users.

[1] K. Lejaeghere, V. Van Speybroeck, G. Van Oost, and S. Cottenier, *Crit. Rev. Solid State* **39**, 1-24 (2014).

[2] K. Lejaeghere, G. Bihlmayer, T. Björkman, P. Blaha, S. Blügel, V. Blum, D. Caliste, I.E. Castelli, S.J. Clark, A. Dal Corso, S. de Gironcoli, T. Deutsch, J.K. Dewhurst, I. Di Marco, C. Draxl, M. Dułak, O. Eriksson, J.A. Flores-Livas, K.F. Garrity, L. Genovese, P. Giannozzi, M. Giantomassi, S. Goedecker, X. Gonze, O. Grånäs, E.K.U. Gross, A. Gulans, F. Gygi, D.R. Hamann, P.J. Hasnip, N.A.W. Holzwarth, D. Iuşan, D.B. Jochym, F. Jollet, D. Jones, G. Kresse, K. Koepnik, E. Küçükbenli, Y.O. Kvashnin, I.L.M. Locht, S. Lubeck, M. Marsman, N. Marzari, U. Nitzsche, L. Nordström, T. Ozaki, L. Paulatto, C.J. Pickard, W. Poelmans, M.I.J. Probert, K. Refson, M. Richter, G.-M. Rignanese, S. Saha, M. Scheffler, M. Schlipf, K. Schwarz, S. Sharma, F. Tavazza, P. Thunström, A. Tkatchenko, M. Torrent, D. Vanderbilt, M.J. van Setten, V. Van Speybroeck, J.M. Wills, J.R. Yates, G.-X. Zhang and S. Cottenier, *Science* **351** (6280), aad3000 (2016).

[3] <http://molmod.ugent.be/deltacodesdft>