Quality control: Has your DFT code been Δ-approved?

Imagine: you and your colleague are both looking for a car. Unaware of each other, you buy exactly the same model on exactly the same day. There is only one difference: yours was made in a German factory, your colleague's in an Austrian one. Do you expect one car to be wider than the other? Of course not.

Now imagine you and your colleague are both looking for the lattice constant of silicon. Unaware of each other, you use exactly the same DFT functional for exactly the same structures. There is only one difference: your code was written by German researchers, your colleague's by Austrian ones. Do you expect one lattice constant to be larger than the other? Yet it is!

The success of density-functional theory (DFT) convinced several research groups to develop their own codes to solve the Kohn-Sham equations. Because each code implements the Kohn-Sham blueprint in slightly different ways, they yield slightly different results. We present an overview of a community-wide effort to assess the agreement between these predictions. Using a quality label Δ, we prove the equivalence of recent DFT codes and potentials, and warn against deprecated ones.