Comparing solid state dft codes, basis sets and potentials

- Landmark community-wide study comparing 15 solid-state codes with 40 potentials or basis sets for PBE equations of state of 71 elemental crystals.
- Metric: \( \Delta \) value = the root-mean-square energy difference between the equations of state of the two codes (the energy-versus-volume curve), averaged over all crystals in a purely elemental benchmark set.
- Conclusion: "most of the commonly used codes and methods are now found to predict essentially identical results".

How to verify the precision of density-functional-theory implementations via reproducible and universal workflows

- A dataset of 960 cubic crystal structures from elements with \( Z = 1 \) to 96, including unaries and oxides across a range of coordination numbers and oxidation states.
- Comparing two all electron codes and a range of pseudopotential-based codes.
- Metric: Birch–Murnaghan parameters of the equations of state of the two codes.
- Conclusion: "AiiDA common workflows perform automatic input parameter selection, provide identical input/output interfaces across codes, and ensure full reproducibility".

Mind the implementation!

- "Multiwavelets applied to metal–ligand interactions: Energies free from basis set errors" compares results with GTOs from ORCA to those with MWs from MRChem.
- Initially, the dataset was computed with BP86. Later, realised that the BP86 versions in ORCA and MRChem are not identical leading to several kcal/mol discrepancies in the CBS limit.
- Everything had to be recomputed with PBE.

Reproducibility of density functional approximations: How new functionals should be reported

- The authors are developers of Libxc.
- Problem with DFT implementations – lack of reliable reference data resulting in non-equivalent implementations. Examples discussed: BP86, PW91, PBE, B3LYP, and others.
- Solution: proposed protocol ensuring reproducibility, e.g., using a standard convergence criteria for quadrature grid, making the source code available, etc.

### TABLE I. Exchange energies of the N and Ne atoms for variants of the PBE exchange functional, employing tabulated Hartree–Fock wave functions evaluated with AtomicOrbitals and a 2000 point radial quadrature with the default scheme of Ref. 40. Libxc keywords are used to identify the functionals.

<table>
<thead>
<tr>
<th>Functional</th>
<th>( E_x(N)/E_h )</th>
<th>( E_x(\text{Ne})/E_h )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Libxc</td>
<td></td>
<td></td>
</tr>
<tr>
<td>gga_x_pbe</td>
<td>(-3.956,025,7)</td>
<td>(-4.448,308,7)</td>
</tr>
<tr>
<td>gga_x_pbe_mod</td>
<td>(-3.956,028,1)</td>
<td>(-4.448,311,4)</td>
</tr>
<tr>
<td>gga_x_pbe_gaussian</td>
<td>(-3.956,018,1)</td>
<td>(-4.448,300,3)</td>
</tr>
</tbody>
</table>


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**Science** 2016, 351, aad3000.

Mind the implementation!

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Reproducibility in DFT

Discrepancy of each computational approach wrt the average all-electron reference dataset. Central blue – the median, outliers – grey points.