Correction: Analysis of computational models for an accurate study of electronic excitations in GFP (vol 17, pg 2582, 2015)

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Correction: Analysis of computational models for an accurate study of electronic excitations in GFP

Tobias Schwabe,* Maarten T. P. Beerepoot, Jógvan Magnus Haugaard Olsen and Jacob Kongsted


On page 2585, Table 4, the results in the last row are incorrect. The correct values are shown below:

<table>
<thead>
<tr>
<th>$R_{\text{cut}}$</th>
<th>Neutral</th>
<th>Anionic</th>
</tr>
</thead>
<tbody>
<tr>
<td>(all/AmberFF94)</td>
<td># Sites</td>
<td>$E_{\text{exc}}$</td>
</tr>
<tr>
<td>3991</td>
<td>3.48</td>
<td>3992</td>
</tr>
</tbody>
</table>

These revised values do not affect any conclusions drawn in our paper. In fact, the absolute excitation energies of the corrected AMBER potential are even closer to the results obtained with the PE(M2P0) potential and underline the observation that neglect of polarization leads to blue-shifted results.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.