



Cite this: *Phys. Chem. Chem. Phys.*,
2016, **18**, 1349

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

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DOI: 10.1039/c5cp90225h

Correction for 'Analysis of computational models for an accurate study of electronic excitations in GFP' by Tobias Schwabe *et al.*, *Phys. Chem. Chem. Phys.*, 2015, **17**, 2582–2588.

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

Table 4 PERI-CC2/def2-TZVP excitation energies (E_{exc}) and relative shift of the neutral and anionic state for increasing GFP truncation model size, characterised by their cut-off radius (R_{cut}) and the number of MM sites (# sites), up to the whole protein model. Distances in Å, energies in eV

| R_{cut} | Neutral | | Anionic | | Shift |
|------------------|---------|------------------|---------|------------------|-------|
| | # Sites | E_{exc} | # Sites | E_{exc} | |
| (all/AmberFF94) | 3991 | 3.48 | 3992 | 2.90 | −0.58 |

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.

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