PCCP



View Article Online

CORRECTION



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

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

Tobias Schwabe,** Maarten T. P. Beerepoot,
b Jógvan Magnus Haugaard Olsen^{\rm cd} and Jacob Kongsted^{\rm d}

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.

www.rsc.org/pccp

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

	Neutral		Anionic		
R _{cut}	# Sites	E _{exc}	# Sites	E _{exc}	Shift
(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.

^a Center for Bioinformatics and Physical Chemistry Institute, Bundesstraße 43, D-22148 Hamburg, Germany. E-mail: schwabe@zbh.uni-hamburg.de;

Fax: +49 40 42838 7352; Tel: +49 40 42838 7333

^b Centre for Theoretical and Computational Chemistry, Department of Chemistry, University of Tromsø – The Arctic University of Norway, N-9037 Tromsø, Norway

^c Laboratory of Computational Chemistry and Biochemistry, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

^d Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, DK-5230 Odense, Denmark