## **PCCP**



## CORRECTION

View Article Online
View Journal | View Issue



Cite this: Phys. Chem. Chem. Phys., 2018, 20, 17530

## Correction: Connectivity dependence of Fano resonances in single molecules

Ali K. Ismael, ab lain Grace and Colin J. Lambert\*

Correction for 'Connectivity dependence of Fano resonances in single molecules' by Ali K. Ismael *et al.*, *Phys. Chem. Chem. Phys.*, 2017, **19**, 6416–6421.

DOI: 10.1039/c8cp91790f

rsc.li/pccp

The lines in Fig. 8 are incorrectly labeled. The caption for Fig. 8 should read:

"Fig. 8. DFT transmission curves. (a) The black curve shows the transmission coefficient for molecule b of Fig. 3. (b) The blue dashed curve shows the transmission coefficient for molecule a of Fig. 3."

Therefore, the first two paragraphs of Section III should read:

"So far the discussion has focused on tight-binding representations of the molecules shown in Fig. 7.

For molecules (a and b) containing two carbonyl groups, Fig. 8 shows DFT results for the transmission coefficients (see Methods for more details). In common with the tight binding results of Fig. 4, both a and b show alternating destructive interference features. In the case of a, such a feature occurs between the LUMO and LUMO+1, whereas in the case of b, they occur between the HOMO and LUMO and between LUMO+2 and LUMO+3. On the other hand for both molecules, destructive interference features appear near E = -2.4 eV, which are almost independent of connectivity, signaling the presence of a Fano resonance."

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

 $<sup>^</sup>a$  Department of Physics, Lancaster University, Lancaster, UK. E-mail: c.lambert@lancaster.ac.uk

<sup>&</sup>lt;sup>b</sup> Department of Physics, College of Education for Pure Science, Tikrit University, Tikrit, Iraq