



Correction: Helical orbitals and circular currents in linear carbon wires

Cite this: *Chem. Sci.*, 2020, **11**, 2568

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DOI: 10.1039/d0sc90031a

rsc.li/chemical-science

Correction for 'Helical orbitals and circular currents in linear carbon wires' by Marc H. Garner *et al.*, *Chem. Sci.*, 2019, **10**, 4598–4608.

In the original article, a technical error in our homemade code (available at https://github.com/marchgarner/Current_Density) meant that the diameter of the current density arrows was scaled incorrectly. We state in the original paper that the diameter of each arrow is the vector-length (*i.e.*, the magnitude of the current density \mathbf{j} in position \mathbf{r}). However, it was incorrectly scaled as only the z -component (the transport direction) was considered in the diameter in the originally published figures. This meant that the circular current components were underestimated in the visual presentation, and consequently the circular currents are much clearer and stronger in magnitude than can be deduced from our original presentation.

Here we reproduce all the figures from the original article and ESI material that showed current density plots. The figures are numbered with the same numbers as in the original article. All central conclusions from the original paper remain unchanged, and are in fact further supported by the correct figures, because the circular current components were previously not properly



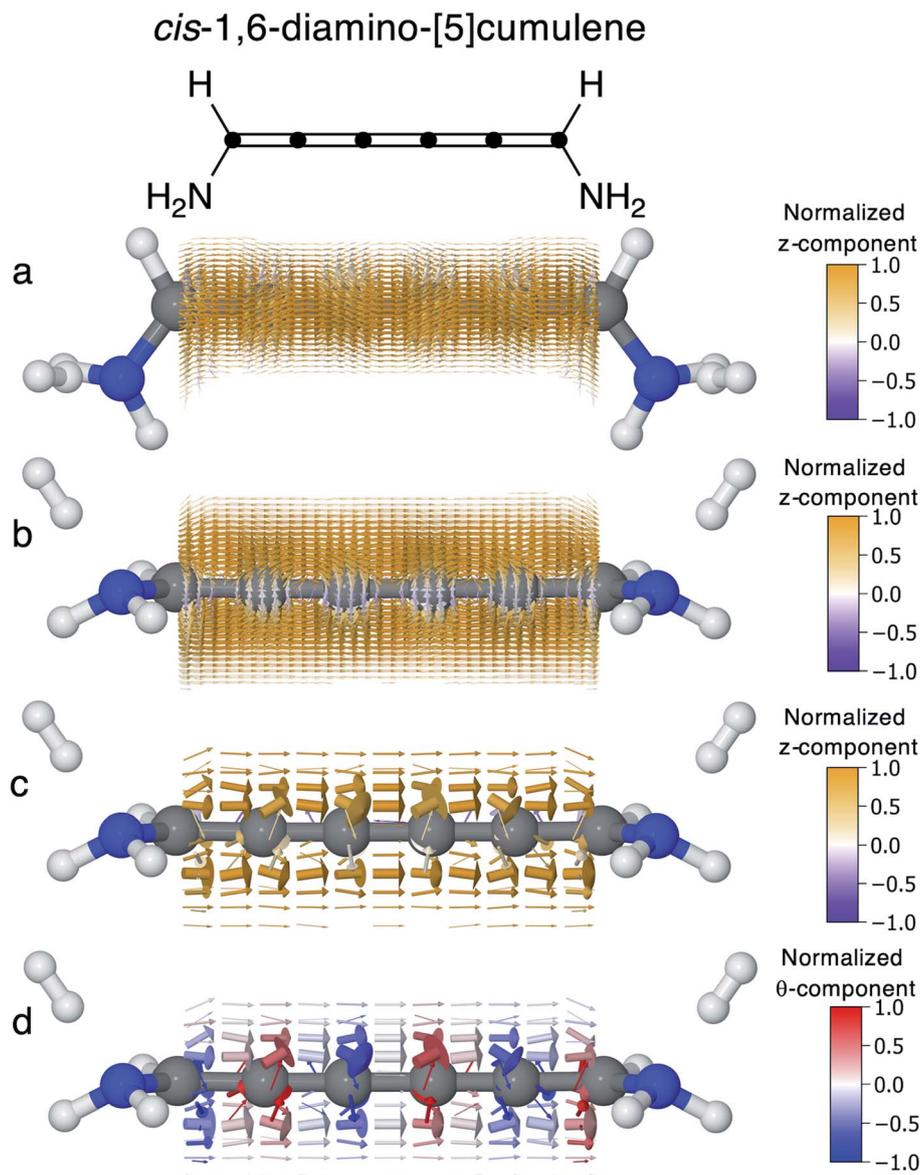


Fig. 6 Current density calculated at the Fermi energy for *cis*-1,6-diamino-[5]cumulene; the 6-carbon cumulene with normal rectilinear π -orbitals. (a) Vector field calculated on a high-density grid and coloured by the z -component shown from top-view. (b) Vector field calculated on a high-density grid and coloured by the z -component shown from side-view, with the nodal plane in the current clearly visible. (c) Vector field calculated on a low-density grid and coloured by the z -component shown from side-view. (d) Vector field calculated on a low-density grid and coloured by the θ -component shown from side-view.

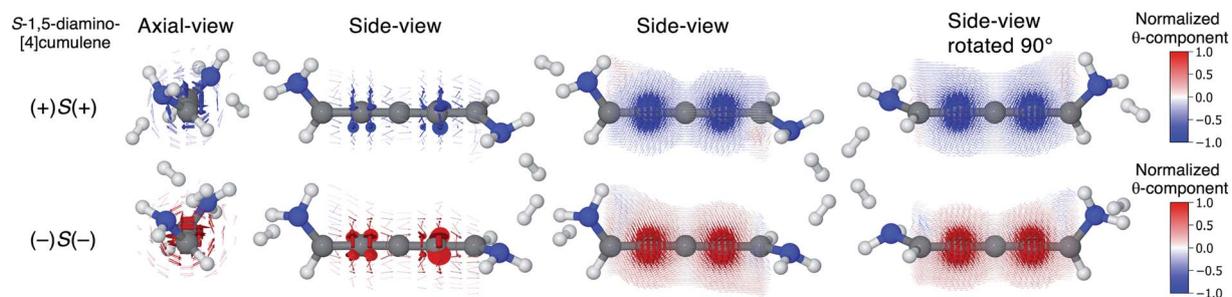


Fig. 7 Current density calculated at the Fermi energy for the (+)*S*(+) and (–)*S*(–) conformations of 1,5-diamino-[4]cumulene. The vector field is shown on both low and high-density grids and is colored by the θ -component.



accounted for in the diameter of the current arrows. In cases where the plots primarily have currents in the z direction (for example Fig. 6) the change in the figures is less pronounced.

In the original article, based on Fig. 7, we noted that there is a nodal plane in the current density, as is also seen for the current in normal π systems (e.g. in Fig. 6). However, this is only true for the z -component of the current density, i.e., the forward current as we plotted previously. With the circular components included this nodal plane is not preserved, as can now be seen in Fig. 7.

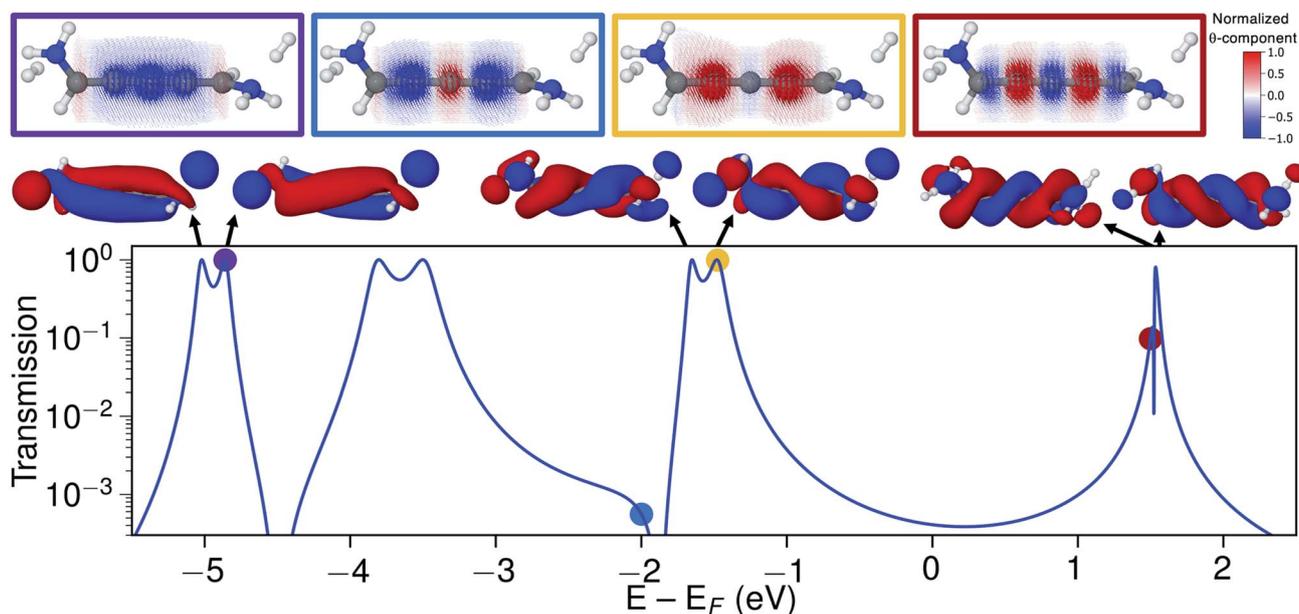


Fig. 8 Transmission calculated with s -band electrodes, molecular orbitals of the junction, and current density calculated at select energies for the $(-S)(-)$ conformation of S -1,5-diamino-[4]cumulene. The current density vector field is shown on a high-density grid and is colored by the θ -component. In the transmission plot, arrows indicate orbital energy (at the corresponding transmission resonances), colored dots indicate the energy at which the current density is calculated.

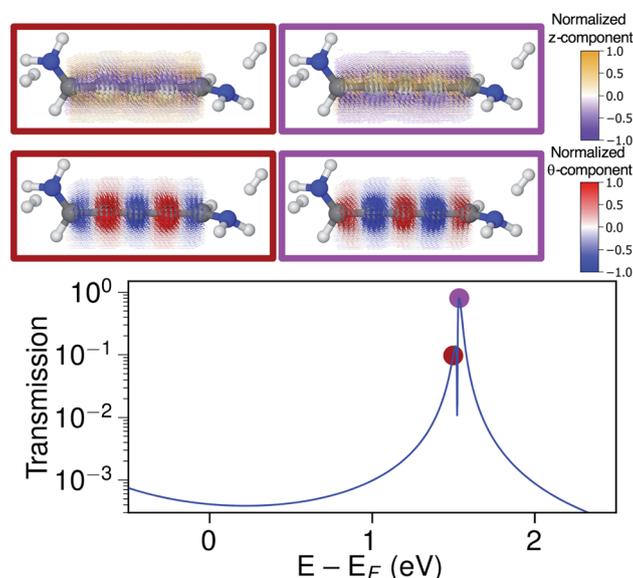


Fig. 9 Transmission calculated with s -band electrodes and current density calculated around the LUMO resonance energy for the $(-S)(-)$ conformation of 1,5-diamino-[4]cumulene. The current density vector field is shown on a high-density grid and is coloured by the z -component (first row) and by the θ -component (second row). In the transmission plot coloured dots indicate the energy at which the current density is calculated.



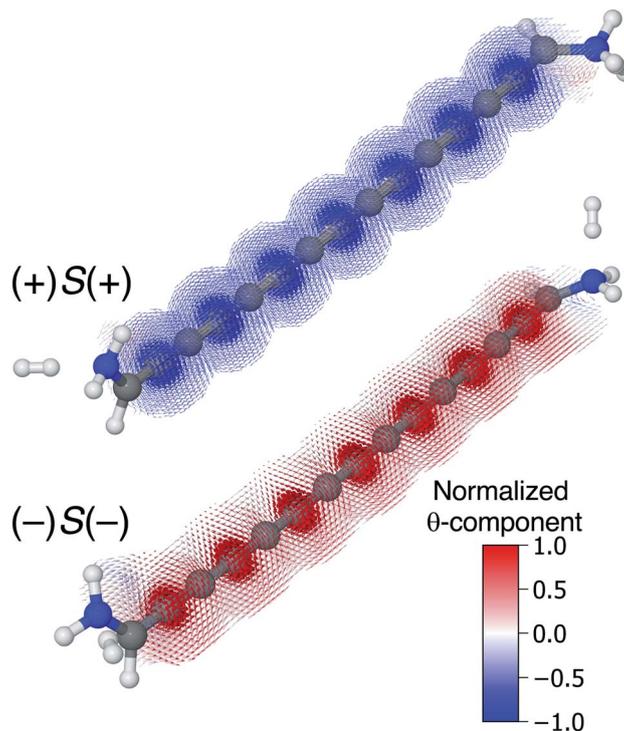


Fig. 10 Current density calculated at the Fermi energy for the (+)S(+) and (-)S(-) conformations of 1,15-diamino-[14]cumulene; the 15-carbon cumulene with helical π -orbitals. The vector field is calculated on a high-density grid and coloured by the θ -component.

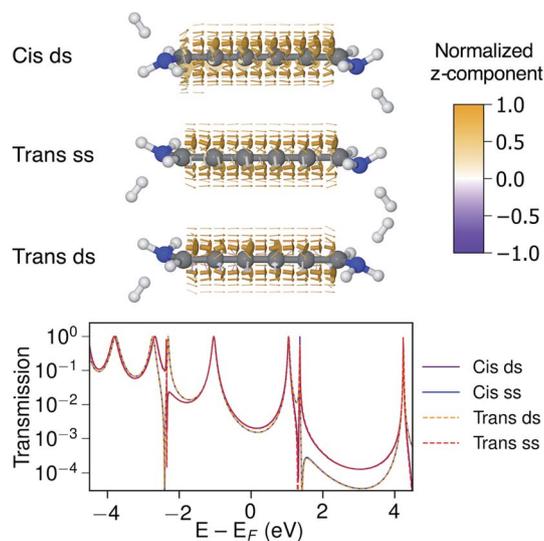


Fig. S9 Current density and transmission of 1,6-diamino-[5]cumulene calculated using wide-band electrodes. The *cis* and *trans* isomers can have lone-pairs pointing to the same side (ss) or to different sides (ds) of the plane of the cumulene. The current density of Cis-ss is shown in Fig. 6 in the manuscript.

Given that we scale the current density arrows in each plot by the largest arrow, it is now clear that in many cases the circular currents can be much larger than the net current. This naturally raises the question as to whether a large magnetic field can be achieved from these ring currents even at a low bias. We are working towards assessing this in the near future.

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

