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CORRECTION

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Correction: Converting benzene into γ-graphyne and its enhanced electrochemical oxygen evolution performance

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Correction for 'Converting benzene into γ-graphyne and its enhanced electrochemical oxygen evolution performance' by Qiaodan Li *et al.*, *J. Mater. Chem. A*, 2019, **7**, 5981–5990, https://doi.org/10.1039/C8TA10317H.

The authors regret errors in the original manuscript in the lattice plane assignment of the lattice fringes in Fig. 2h, the crystal lattices of γ-graphyne in Fig. S3 of the original ESI and in the calculation of bond enthalpies change on page 3 of the original ESI.

The lattice fringes of 0.17 nm (Fig. 2i) and 0.20 nm (Fig. 2h and i) should be assigned to the (220) and (300) lattice planes, respectively, rather than to the (440) and (422) lattice planes stated in the published article. Fig. 2h is revised accordingly.

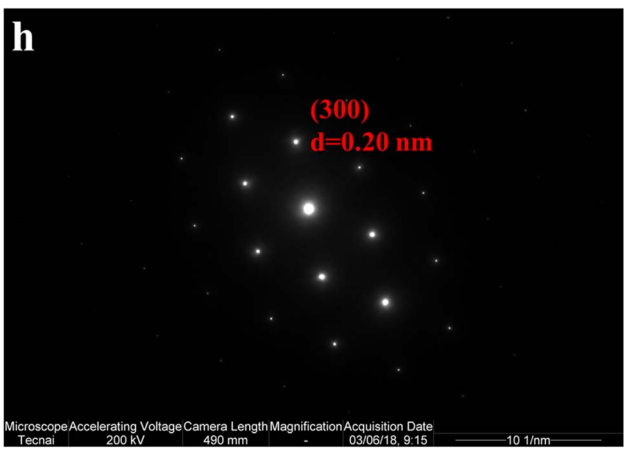

Fig. 2 (h) SAED pattern of the as-prepared γ-graphyne.

In the calculation of the Gibbs free energy change in the ESI, the calculation of bond enthalpies change is incorrect. "$6N/N_A \times (332 - 414) + 3N/N_A \times (-181.5 + 62.8)$" should be corrected to "$6N/N_A \times (-332 + 414) + 3N/N_A \times (-181.5 + 62.8)$". This makes $\Delta G_3 > 0$ ($\Delta G_3 = kN \times [135\,900/R + 260T/R + \ln(64/27)T]$). A hypothetical two-step reaction follows: (1) mechanochemical dehydrogenation of C–H bonds, and (2) a reaction between generated C_6 fragments and CaC_2. Though the first step is non-spontaneous, mechanochemistry is a powerful technology for providing enough of a driving force for the reaction. The second step is spontaneous, as calculated below.

$$\begin{aligned}\Delta H &= H_{\gamma\text{-graphyne}} - H_{C_6} + H_{Ca} - H_{CaC_2}\\ &= \frac{6N}{N_A}\left(E_{C-C(\text{aromatic})} + E_{C-C} - E_{C-C(\text{aromatic})}\right) + \frac{3N}{N_A}\left(\Delta_f H^{\theta}_{Ca} - \Delta_f H^{\theta}_{CaC_2}\right)\\ &= \frac{6N}{N_A}(-332) + \frac{3N}{N_A}(0 + 63)\\ &= -1614\frac{N}{N_A}(\text{kJ})\end{aligned}$$

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$$\begin{aligned}\Delta S &= S_{\gamma\text{-graphyne}} - S_{C_6} + S_{Ca} - S_{CaC_2} + \Delta S_{mix}\\ &= \frac{1}{N_A}\Delta_f S^{\theta}_{\gamma\text{-graphyne}} - \frac{N}{N_A}\Delta_f S^{\theta}_{C_6} + 3\frac{N}{N_A}\left(\Delta_f S^{\theta}_{Ca} - \Delta_f S^{\theta}_{CaC_2}\right) + \Delta S_{mix}\\ &= \frac{1}{N_A}\Delta_f S^{\theta}_{\gamma\text{-graphyne}} - \frac{N}{N_A}\Delta_f S^{\theta}_{C_6} + 3\frac{N}{N_A}(42-70) + k\ln\frac{(3N+1)!}{3N!} - k\ln\frac{(N+3N)!}{(3N)!N!}\\ &= \frac{1}{N_A}\left(\Delta_f S^{\theta}_{\gamma\text{-graphyne}} - \Delta_f S^{\theta}_{C_6}\right) - 84\frac{N}{N_A} + k\ln(3N+1) - 9.5kN\left(\mathrm{J\ K^{-1}}\right)\end{aligned}$$

$$\begin{aligned}\Delta G &= \Delta H - T\Delta S\\ &= -1\,614\,000\frac{N}{N_A} - \frac{T}{N_A}\left(\Delta_f S^{\theta}_{\gamma\text{-graphyne}} - \Delta_f S^{\theta}_{C_6}\right) + 84\frac{NT}{N_A} - kT\ln(3N+1) + 9.5kNT\\ &= -\frac{T}{N_A}\left(\Delta_f S^{\theta}_{\gamma\text{-graphyne}} - \Delta_f S^{\theta}_{C_6}\right) - kT\ln(3N+1) - \frac{N}{N_A}(1\,614\,000 - 84T - 9.5RT)\end{aligned}$$

when $T < 9903$ K, and $\Delta G < 0$.

The updated Fig. S3 is shown below.

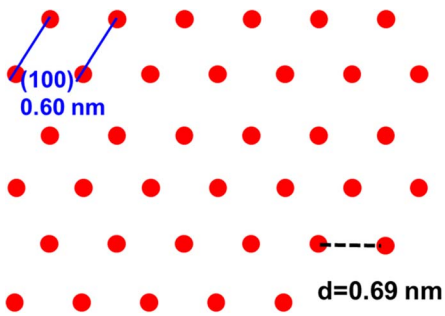

Fig. S3 The crystal lattices of γ-graphyne.

An independent expert has viewed the corrected Fig. 2h, Fig. S3 and the corrections to the calculation of bond enthalpies change, and confirmed that they are consistent with the discussions and conclusions presented.

An 'Update to the Supplementary information' with the updated calculation of bond enthalpies and Fig. S3 has been published accordingly as a separate document.

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

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