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CORRECTION

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Correction: Graph neural network based coarse-grained mapping prediction

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Correction for 'Graph neural network based coarse-grained mapping prediction' by Zhiheng Li *et al.*, *Chem. Sci.*, 2020, **11**, 9524–9531, DOI: 10.1039/D0SC02458A.

The authors regret that eqn (5) was missing the adjacency matrix term. The correct form of eqn (5) is shown below:

$$A_{ij} = \exp\left(\frac{-\|\tilde{X}_i - \tilde{X}_j\|_2^2}{2\sigma^2}\right)\tilde{E}, \tag{5}$$

where σ is the bandwidth and is set to $\sigma = 1$ in the experiment. $\tilde{E} \in \mathbb{R}^{n\times n}$ denotes the adjacency matrix ($\tilde{E}_{ij} = 1$ if atom i and atom j are bonded, otherwise $\tilde{E}_{ij} = 0$).

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

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