

## CORRECTION

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**Correction: Graph neural network based coarse-grained mapping prediction**Zhiheng Li,<sup>a</sup> Geemi P. Wellawatte,<sup>b</sup> Maghesree Chakraborty,<sup>c</sup> Heta A. Gandhi,<sup>c</sup> Chenliang Xu<sup>\*a</sup> and Andrew D. White<sup>\*c</sup>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:

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

where  $\sigma$  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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