



Correction: Graph neural network based coarse-grained mapping prediction

Cite this: *Chem. Sci.*, 2021, 12, 11922

Zhiheng Li,^a Geemi P. Wellawatte,^b Maghesree Chakraborty,^c Heta A. Gandhi,^c Chenliang Xu^{*a} and Andrew D. White^{*c}

DOI: 10.1039/d1sc90186a

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.

rsc.li/chemical-science

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 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.

^aDepartment of Computer Science, University of Rochester, USA

^bDepartment of Chemistry, University of Rochester, USA

^cDepartment of Chemical Engineering, University of Rochester, USA. E-mail: andrew.white@rochester.edu

