



Cite this: *Phys. Chem. Chem. Phys.*, 2021, **23**, 8936

Correction: Analysis and visualization of energy densities. I. Insights from real-time time-dependent density functional theory simulations

Junjie Yang,^a Zheng Pei,^b Jingheng Deng,^a Yuezhi Mao,^c Qin Wu,^d Zhibo Yang,^a Bin Wang,^e Christine M. Aikens,^f Wanzhen Liang^{*b} and Yihan Shao^{*a}

DOI: 10.1039/d1cp90057a

rsc.li/pccp

Correction for 'Analysis and visualization of energy densities. I. Insights from real-time time-dependent density functional theory simulations' by Junjie Yang *et al.*, *Phys. Chem. Chem. Phys.*, 2020, **22**, 26838–26851, DOI: 10.1039/d0cp04206d.

The published version of this manuscript included an error in eqn (A6). The correct equation is shown below:

$$\mathbf{U}(t) = \begin{pmatrix} \mathbf{I}_{oo} & -\boldsymbol{\Theta}^\dagger(t) \\ \boldsymbol{\Theta}(t) & \mathbf{I}_{vv} \end{pmatrix} + \mathcal{O}(\boldsymbol{\Theta}^2) \quad (1)$$

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



^a Department of Chemistry and Biochemistry, University of Oklahoma, 101 Stephenson Pkwy, Norman, OK 73019, USA. E-mail: yihan.shao@ou.edu

^b State Key Laboratory of Physical Chemistry of Solid Surfaces, Collaborative Innovation Center of Chemistry for Energy Materials, Fujian Provincial Key Laboratory of Theoretical and Computational Chemistry, and Department of Chemistry, College of Chemistry and Chemical Engineering, Xiamen University, Xiamen 361005, P. R. China. E-mail: liangwz@xmu.edu.cn

^c Department of Chemistry, Stanford University, Stanford, CA 94305, USA

^d Center for Functional Nanomaterials, Brookhaven National Laboratory, Upton, NY 11973, USA

^e Center for Interfacial Reaction Engineering and School of Chemical, Biological, and Materials Engineering, Gallogly College of Engineering, University of Oklahoma, Norman, OK 73019, USA

^f Department of Chemistry, Kansas State University, Manhattan, KS 66506, USA