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CORRECTION

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Correction: First-principles modeling of the highly dynamical surface structure of a MoS_2 catalyst with S-vacancies

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Correction for 'First-principles modeling of the highly dynamical surface structure of a MoS_2 catalyst with S-vacancies' by Po-Yuan Wang *et al.*, *Phys. Chem. Chem. Phys.*, 2022, **24**, 24166–24172, https://doi.org/10.1039/D2CP03384D.

The authors have recently discovered an error that affects the barriers (E_a) of one diffusion process and reaction energies (E_r) of two diffusion processes in the published version of the manuscript. However, the error does not affect the general conclusion of the work, as outlined below. The authors had unintentionally misplaced one atom during the geometry optimization of a minimum structure, the initial state for the diffusion process 1o2o3o4o5o6x7x8o (corrected geometry provided in the ESI of the original paper), which led to this error. The corrected E_a and E_r values for the affected processes are, together with the data originally published in Table S1 of the ESI, shown in Table 1.

Table 1 Originally published and corrected reaction energies (E_r) and diffusion barriers (E_a) for the affected diffusion processes in the forward direction. All values are given in eV. The values that have changed in the present correction are marked in bold

	Original		Corrected	
Diffusion process	E_r	E_a	E_r	E_a
1x2x3o4o5o6o7o8o	−0.53	0.91	**−0.31**	0.91
1o2o3o4o5o6x7x8o	0.53	1.44	**0.31**	**1.22**

Fig. 1 below, corresponding to Fig. 2(a) in the original paper, shows the correlation between the E_a and E_r values of the investigated diffusion steps. It can be seen that the claim that low diffusion barriers are associated with an S-vacancy on Site 5 is unaffected by the error above. The linear scaling relations between the E_a and E_r values reported originally are only minimally affected: When only considering the diffusion processes that feature S-vacancies on both Site 4 and Site 5, the linear scaling relation changes from $E_a = 0.05 \times E_r + 1.02$ eV to $E_a = 0.05 \times E_r + 1.01$ eV. When accounting for all diffusion processes with an S-vacancy on Site 5, the relation remains $E_a = 0.05 \times E_r + 0.97$ eV, the same as in the original paper.

In the next few lines, the authors have illustrated that the changed energetics do not affect the kinetic modeling results. The affected diffusion processes feature six S-vacany sites around the initial or final position of the diffusing S-vacancy. This means the kinetic Monte Carlo (kMC) simulation results for the diffusion of 5S-vacancies and systems involving fewer S-vacancies are all unaffected. Similarly, the simulation starting from the MoS_2 surface with randomly distributed S-vacancies is also unlikely to change due to the changed energetics, as the system does not feature any region with a sufficiently high concentration of defect sites in which the mentioned diffusion processes would be relevant. The only systems that had to be reconsidered are those kMC simulations starting from large, connected *n*S-vacancies, as shown in Fig. 5(d), Fig. S11(b), Fig. S12(b), and Fig. S13(b) of the original publication. The corresponding simulations have been rerun with the updated data and are shown in Fig. 2. The differences are insignificant, indicating that the error in the E_a and E_r values does not affect the kinetic simulations of the original publication, and with that, also none of its conclusions.

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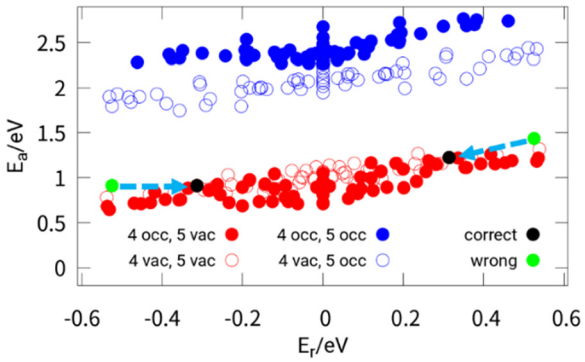

Fig. 1 This figure corresponds to Fig. 2(a) in the original paper and shows the calculated E_a and reaction energies E_r for the diffusion of a single S-vacancy. The color/filling of the data points indicates whether specific sites are empty/occupied. The wrong data points published in the original paper are marked in green, and the corrected data points are in black.

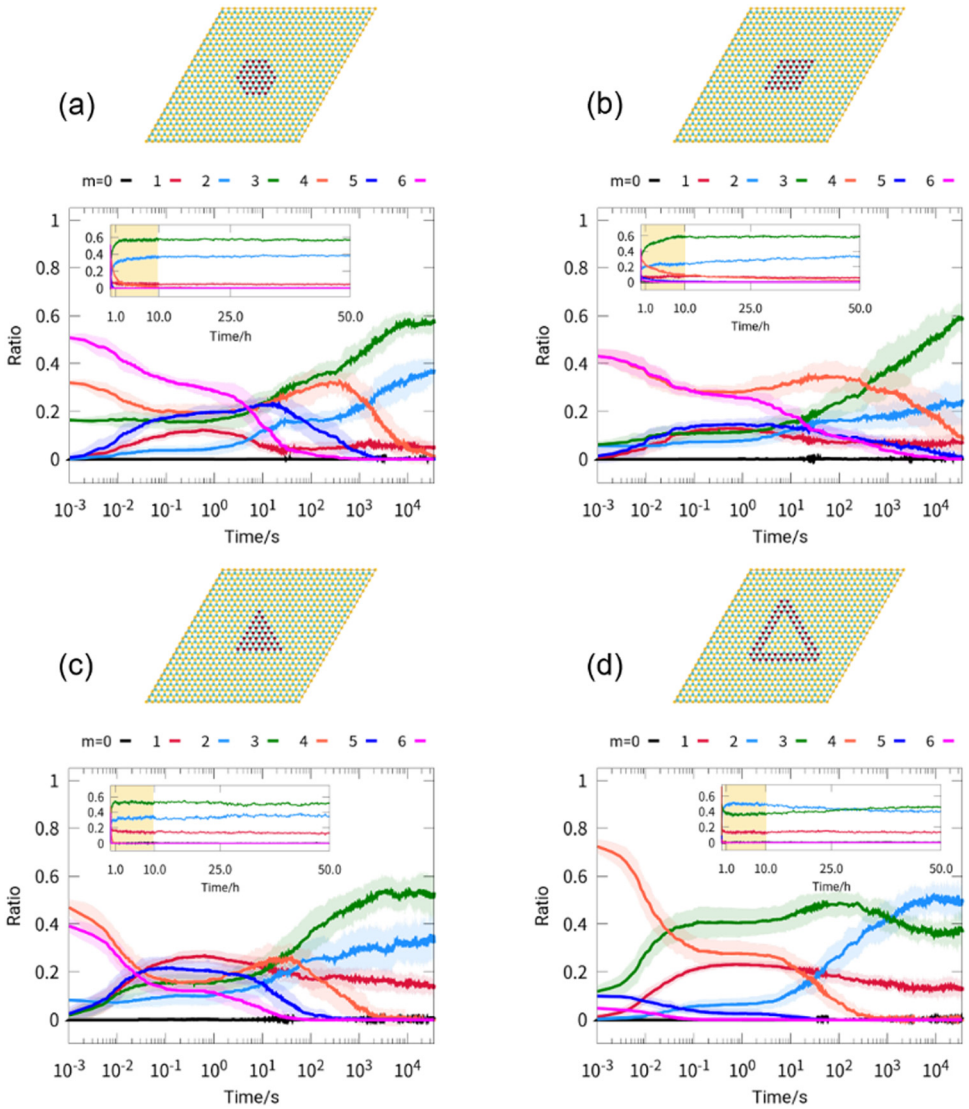

Fig. 2 Part (a) corresponds to Fig. 5(d) of the original paper; (b)–(d) refer to Fig. S11(b), Fig. S12(b), and Fig. S13(b) of the ESI of the original paper. The figures show the ratio of S-vacancies with m neighboring S-vacancy sites as a function of time and initial geometry, which is displayed at the top of each figure. All shown data are obtained by averaging over 32 kMC simulations under identical conditions. The background of the curves in a lighter color marks the standard deviation.

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

