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CORRECTION

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Correction: Penetrating probability and cross section of the Li^+–C_{60} encapsulation process through an *ab initio* molecular dynamics investigation

Thi H. Ho,[ab] Yoshiyuki Kawazoe[c] and Hung M. Le*[d]

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Correction for 'Penetrating probability and cross section of the Li^+–C_{60} encapsulation process through an *ab initio* molecular dynamics investigation' by Thi H. Ho *et al.*, *Phys. Chem. Chem. Phys.*, 2018, **20**, 7007–7013.

We would like to make readers aware of a paper by Ohno *et al.*[1] which was published while this manuscript was under review, and clarify the differences between the results obtained by the two studies.

We performed statistical molecular dynamics (MD) simulations for the collision between Li^+ and a targeted six-membered ring in C_{60}. The purpose of this investigation, in a clear context, is to determine the penetrating probability of Li^+ through the targeted six-membered ring statistically, as described in detail in Fig. 1 of the original paper. The target point of the collision was chosen randomly within a radius of 0.5 Å. As a result of firing directly toward a six-membered ring, the penetrating probability was up to 15.6% with the starting Li^+ kinetic energy of 15 eV. When the kinetic energy was 9 eV, the penetrating probability was 5.4%. Our penetrating probability was much higher than that obtained by Ohno *et al.*[1]

In their investigation, Ohno *et al.*[1] set up firing cases in which Li^+ struck a hexagonal six-membered ring (or pentagonal five-membered ring) with a chosen incidence angle (varied from 0° to 42°) and a defined impinging point (from −1 Å to 1 Å from the hexagonal-ring center). Therefore, their study represents a detailed survey of the most available striking cases, from which the reaction probability was derived. Their results, unsurprisingly, indicated that it was difficult for Li^+ to get through the barrier to form $Li^+@C_{60}$. For example, with an incident kinetic energy of 10 eV, the penetrating probability was only 1.3%. Moreover, in many cases, severe deformation (or destruction) of the C_{60} cage was observed.

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

References

1 K. Ohno, A. Manjanath, Y. Kawazoe, R. Hatakeyama, F. Misaizu, E. Kwon, H. Fukumura, H. Ogasawara, Y. Yamada, C. Zhang, N. Sumi, T. Kamigaki, K. Kawachi, K. Yokoo, S. Onoi and Y. Kasama, *Nanoscale*, 2018, **10**, 1825–1836.

[a] *Division of Computational Physics, Institute for Computational Science, Ton Duc Thang University, Ho Chi Minh City, Vietnam. E-mail: hohuynhthi@tdt.edu.vn*
[b] *Faculty of Applied Sciences, Ton Duc Thang University, Ho Chi Minh City, Vietnam*
[c] *New Industry Creation Hatchery Center, Tohoku University, Sendai, 980-8579, Japan*
[d] *Division of Molecular Modeling, Center for Innovative Materials and Architectures, Vietnam National University, Ho Chi Minh City, Vietnam. E-mail: hung.m.le@hotmail.com*