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## Correction: Infrared spectroscopy for understanding the structure of Nafion and its associated properties

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Correction for 'Infrared spectroscopy for understanding the structure of Nafion and its associated properties' by Tanya Agarwal *et al.*, *J. Mater. Chem. A*, 2024, <https://doi.org/10.1039/D3TA05653H>.

The authors regret that the original article contained some misinterpretations of two cited publications, which they have since been made aware of in conversation with the authors of said works. As such, amendments to the main article text need to be made in the following locations – first, with regards to ref. 36 (reproduced here as ref. 1):

1. Section 3.1.1/paragraph 1

*Original text:* “Density Functional Theory (DFT) calculations performed using X3LYP exchange correlation functional taking  $\lambda = 3$  show that  $1060\text{ cm}^{-1}$  is dominated by the asymmetric stretching of the side chain ether group coupled to  $\text{SO}_3^-$  symmetric stretching in agreement with findings of other groups.”

*Correction:* “Density Functional Theory (DFT) calculations performed using X3LYP exchange correlation functional show that  $1060\text{ cm}^{-1}$  is dominated by the asymmetric stretching of the side chain ether group coupled to  $\text{SO}_3^-$  symmetric stretching in agreement with findings of other groups.”

2. Section 3.1.2/paragraph 2

*Original text:* “Webber *et al.*...that the groups at  $983\text{ cm}^{-1}$  and  $970\text{ cm}^{-1}$  were dominated by  $-\text{SO}_3^-$  symmetric stretching coupled to the ether group mode.”

*Correction:* “Webber *et al.*...that the experimentally observed  $970\text{ cm}^{-1}$  band is dominated by  $-\text{SO}_3^-$  symmetric stretching coupled to the ether group mode.”

3. Section 3.1.2/paragraph 4

*Original text:* “The  $980\text{ cm}^{-1}$  mode was not found to change much with hydration. This indicates that the  $980\text{ cm}^{-1}$  mode might not be dominated by the  $-\text{SO}_3^-$  symmetric stretching as calculated by Webber *et al.* and others.”

*Correction:* “The  $980\text{ cm}^{-1}$  mode was not found to change much with hydration: the COC group, tethered to the backbone, does not have internal coordinates that are mechanically coupled to the distant  $-\text{SO}_3^-$  group.”

Second, with regards to ref. 39 (reproduced here as ref. 2):

4. Section 3.1.1/paragraph 1

*Original text:* “Loupe *et al.* found  $1060\text{ cm}^{-1}$  to be dominated by the C–O–C mode based on their DFT calculations for  $\lambda = 4$ .”

*Correction:* “Loupe *et al.* found  $1060\text{ cm}^{-1}$  to be dominated by the C–O–C mode based on their DFT calculations.”

5. Fig. 8 caption

*Original text:* “DFT calculated spectra for fully dehydrated (blue) and fully hydrated membrane (red).”

*Correction:* “Transmission FTIR spectra for fully dehydrated (blue) and fully hydrated Nafion-H 212 (red).”

6. Section 3.1.2/paragraph 4

*Original text:* “The modes at  $910\text{ cm}^{-1}$ , and  $970\text{ cm}^{-1}$  were found to be a strong function of hydration with  $C_1$  (single functional group mode) dominating below  $\lambda = 3$  and  $C_{3V}$  (three-fold local symmetry) dominating above it.”

*Correction:* “The bands at  $910$  ( $C_1$  mode) and  $970$  ( $C_{3V}$  mode)  $\text{cm}^{-1}$  were found to be a strong function of hydration.  $C_1$  modes refer to the  $\text{SO}_3\text{H}$  group with no local symmetry.  $C_{3V}$  modes refer to the  $\text{SO}_3^-$  group with three-fold symmetry”.

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

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## References

- 1 M. Webber, N. Dimakis, D. Kumari, M. Fuccillo and E. S. Smotkin, Mechanically Coupled Internal Coordinates of Ionomer Vibrational Modes, *Macromolecules*, 2010, **43**(13), 5500–5502, DOI: [10.1021/ma100915u](https://doi.org/10.1021/ma100915u).
- 2 N. Loupe, K. Abu-Hakme, S. Gao, L. Gonzalez, M. Ingargiola, K. Mathiowetz, R. Cruse, J. Doan, A. Schide, I. Salas, N. Dimakis, S. S. Jang, W. A. Goddard III and E. S. Smotkin, Group Vibrational Mode Assignments as a Broadly Applicable Tool for Characterizing Ionomer Membrane Structure as a Function of Degree of Hydration, *Chem. Mater.*, 2020, **32**(5), 1828–1843.

