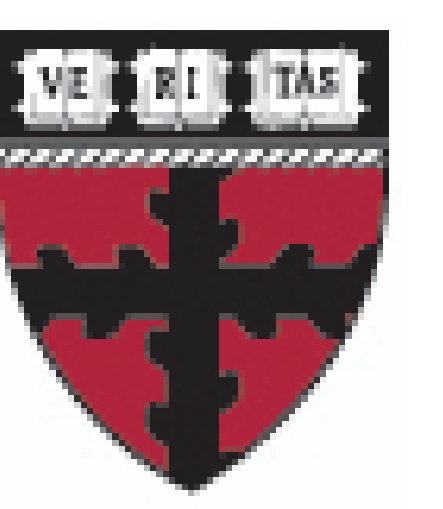


Electrifying Industrial Hydrogen Peroxide Production

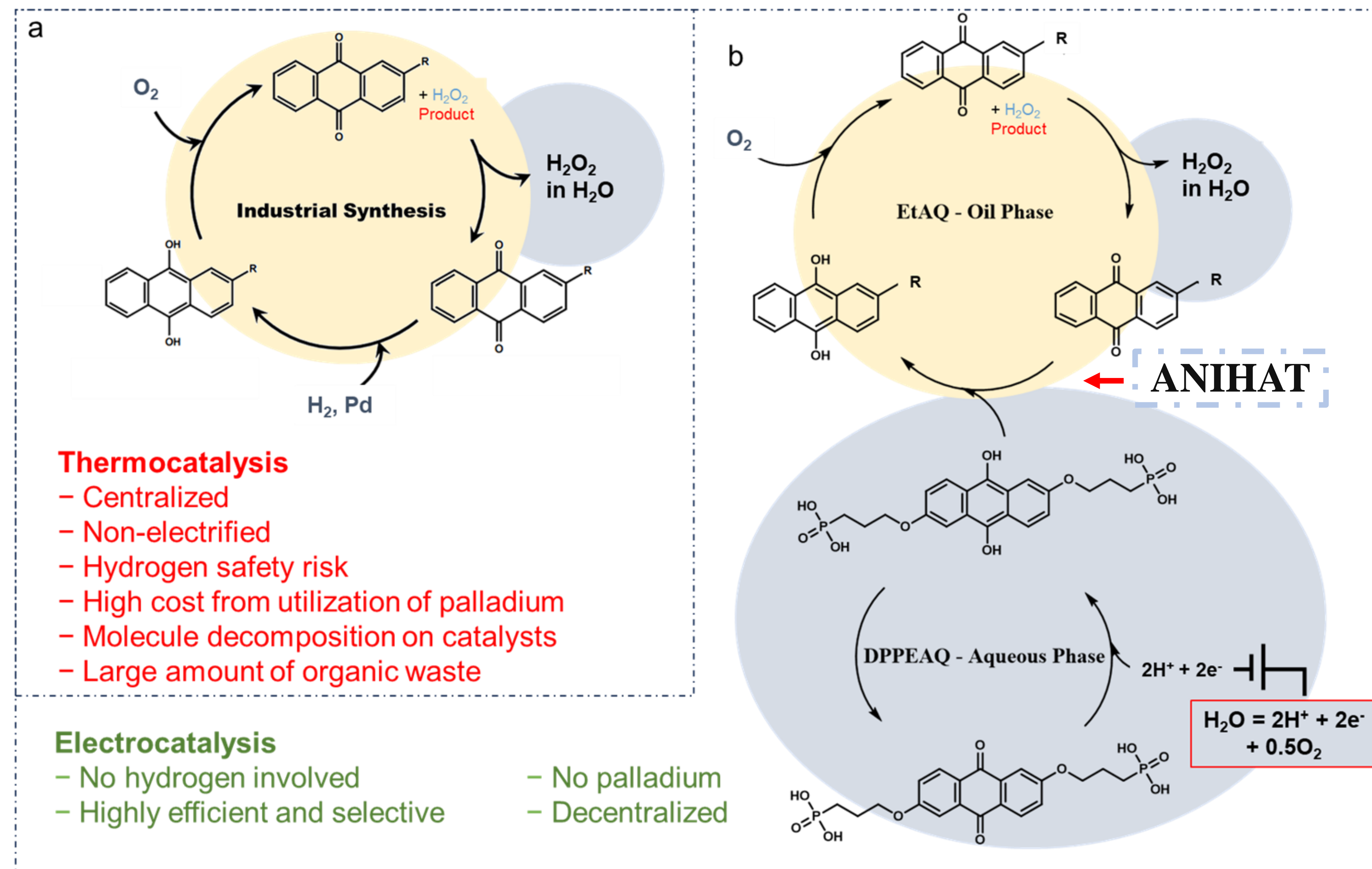
Dawei Xi^{1, #}, Yuheng Wu^{1, #}, Michael J. Aziz¹ *

¹Harvard John A. Paulson School of Engineering and Applied Sciences



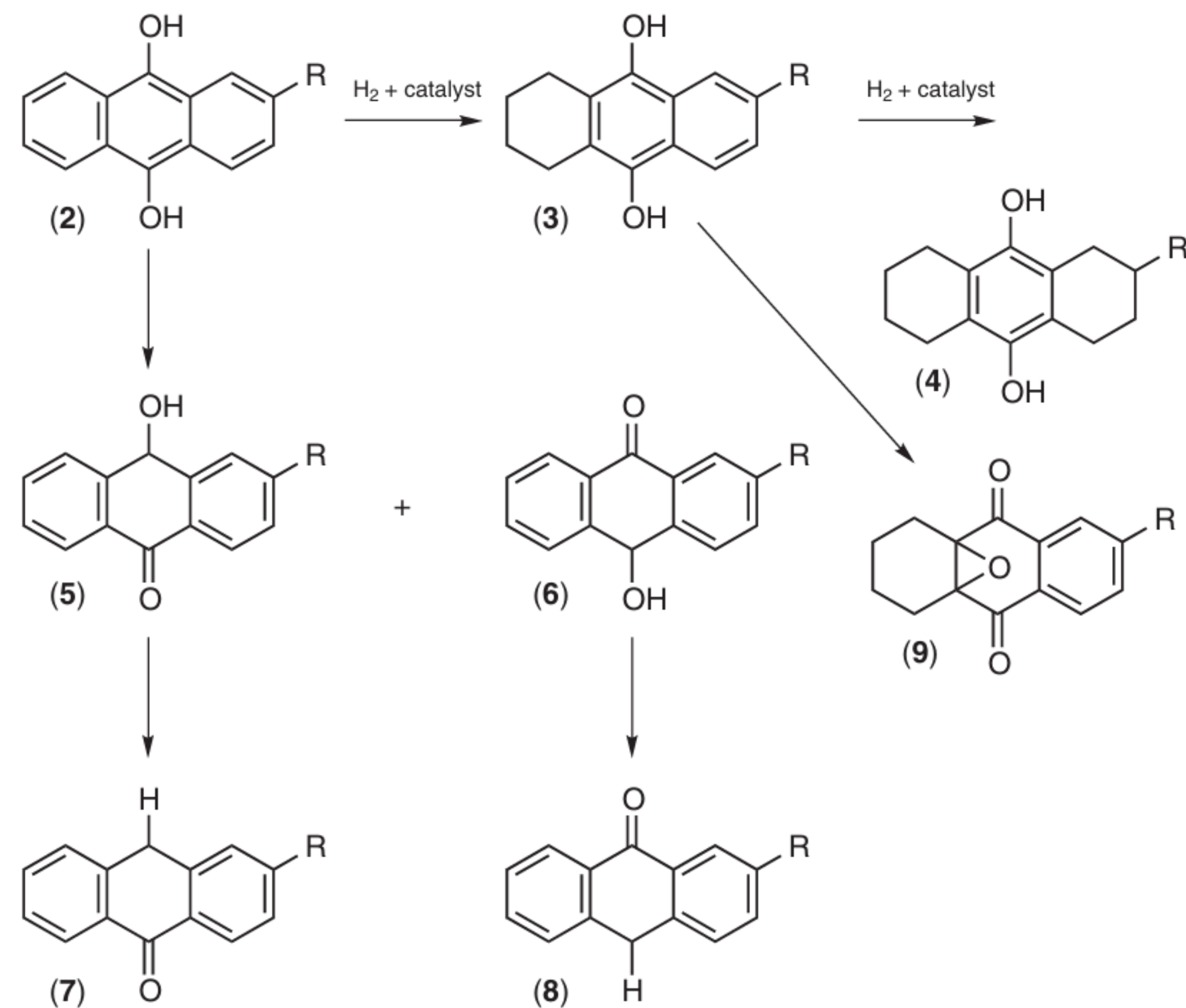
Abstract: Annual global H₂O₂ production is 5 million tons, leading to 15 million tons of CO₂ emissions. The industrial anthraquinone autoxidation (AO) method is the dominant production technology, but it involves high risks of pressurized hydrogen and air input, and requires expensive palladium-based catalysts that can reduce anthraquinone to non-reactive molecules. A considerable amount of energy also has to be put into the distillation and transportation of H₂O₂, providing an opportunity for decentralized electrochemical H₂O₂ production methods. We developed an interface hydrogen atom transfer reaction between an aqueous and a non-aqueous phase to electrify the industrial H₂O₂ production process, avoiding the undesired side-reactions of anthraquinone reduction. The aqueous electrochemical process enables us to produce H₂O₂ with high Faradaic efficiency (>80%) under high current densities (>200 mA cm⁻²). The system can be free of hydrogen gas and noble metal. The H₂O₂ produced this way can be at high concentration (>10%) and free of electrolyte. This method can facilitate the electrification and decentralization of industrial H₂O₂ production, reducing the major capital cost associated with the decomposition of anthraquinone molecules and major energy cost associated with concentrating and transporting H₂O₂.

Comparison between current industrial H₂O₂ production and our electrochemical method

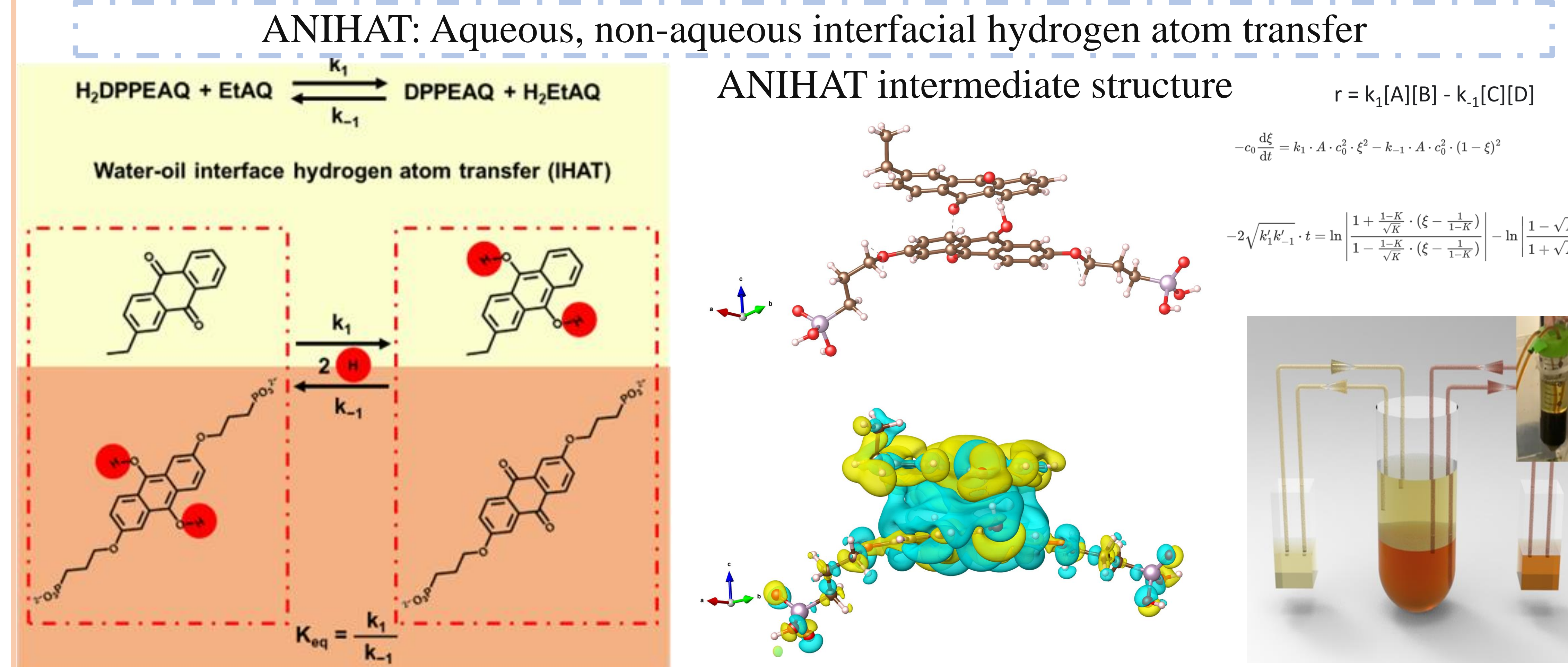


Real pain point for current industrial H₂O₂ production

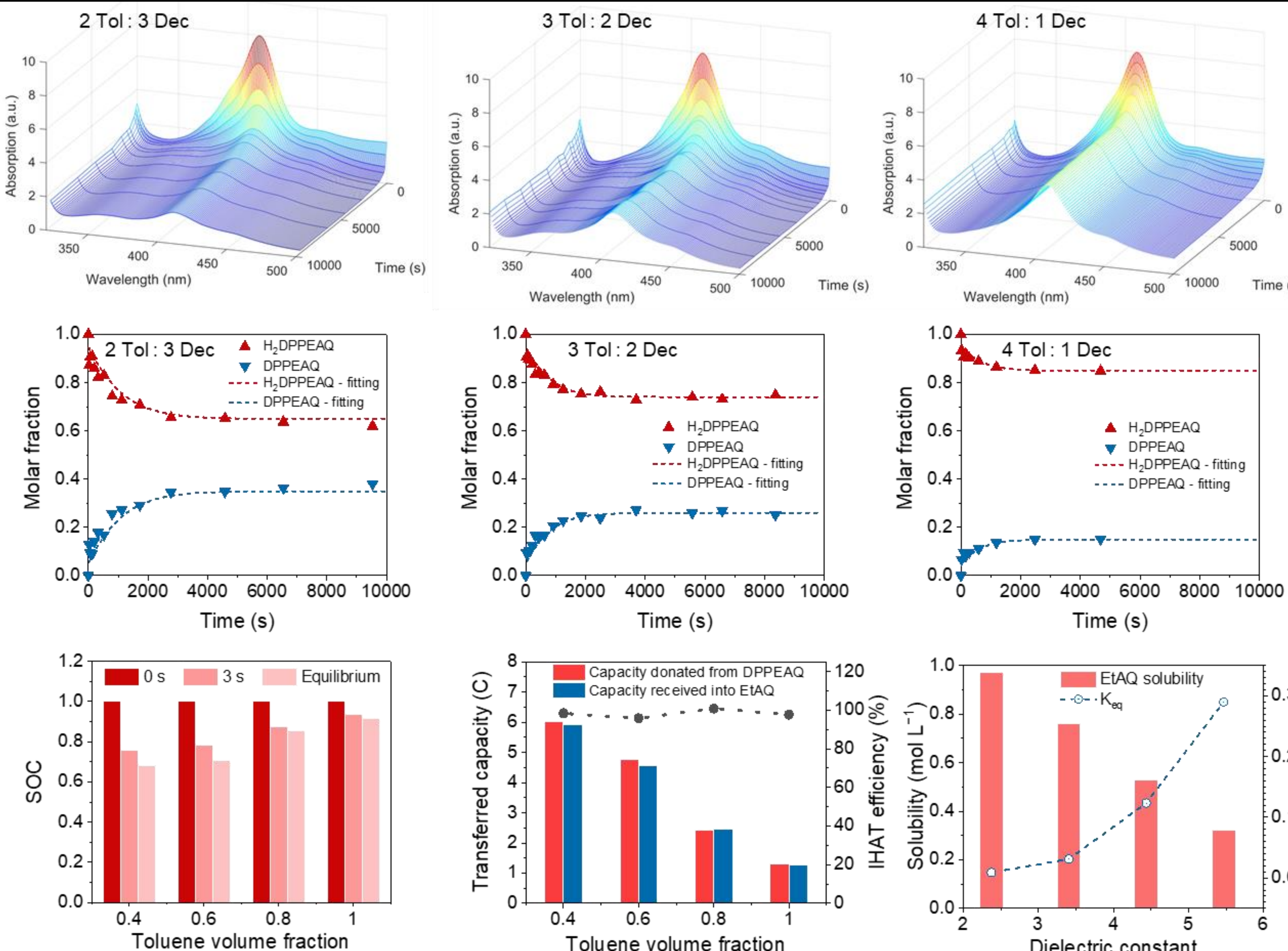
- Hydrogenation selectivity.
- Utilization of solvent with high polarity.
- High polarity solvents are used to help the selectivity and efficiency of hydrogenation.
- Both introduce large amount of organic wastes.



ANIHAT for non-aqueous hydrogenation

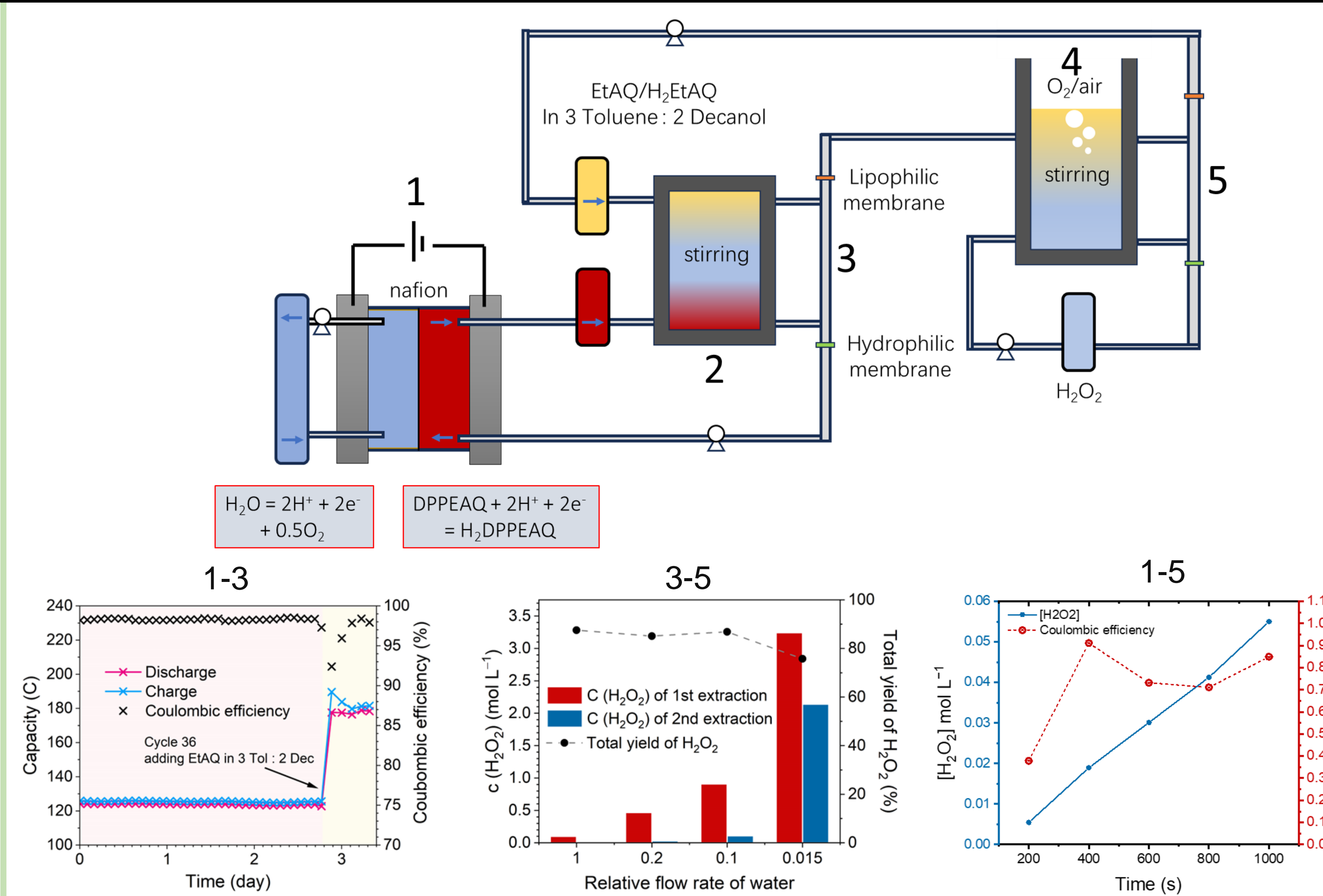


Thermodynamic and kinetic of ANIHAT



- ANIHAT is generally fast interfacial reaction.
- ANIHAT is highly efficient and selective.
- Organic solvent polarity mainly affects the thermodynamic of ANIHAT by influencing the redox potential of non-aqueous anthraquinones.

Integrated systems



Conclusions:

- With various molecules and solvents, the ANIHAT can be > 99% selectivity and Faradaic efficiency, with a current density higher than 0.5 A cm⁻². Overall peroxide efficiency is ~80%.
- With various cell structures and counter reactions, we can do noble metal free, hydrogen gas free pure hydrogen peroxide production.
- With further molecular development, heavy aromatic solvent can be directly used, cutting organic wastes during production.

References:

1. Murray, A. T., Voskian, S., Schreier, M., Hatton, T. A., & Surendranath, Y. (2019). *Joule*, 3(12), 2942-2954.
2. Berlinguette, C. P., et al. "Indirect H₂O₂ synthesis without H₂." (2023).
3. Xia, C., Xia, Y., Zhu, P., Fan, L., & Wang, H. (2019). *Science*, 366(6462), 226-231.
4. Huang, A., Delima, R. S., ... Berlinguette, C. P. (2022). *Journal of the American Chemical Society*, 144(32), 14548-14554.
5. Freakley, S. J., He, Q., Harhry, J. H., ... Hutchings, G. J. (2016). *Science*, 351(6276), 965-968.
6. Hess, Wayne T. "Hydrogen peroxide." *Kirk-Othmer Encyclopedia of Chemical Technology* (2000).

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