Short Communication

First Principles Design of Anthraquinone Derivatives in Redox Flow Batteries

Liangliang Chen¹, Chengwei Ma¹, Xin Li^{1,*}, Luyin Lin^{2,*}, Shengsian Yang², Ge Li¹

¹ School of Chemistry and Chemical Engineering, Beijing Institute of Technology, 100081, Beijing, China

² Department of Chemical Engineering and Biotechnology, National Taipei University of Technology (Taipei Tech), Taipei, 10608, Taiwan

*E-mail: klkxlx@163.com, lylin@mail.ntut.edu.tw

Liangliang Chen and Chengwei Ma contributed equally to this work.

doi: 10.20964/2017.11.35

Received: 20 July 2017 / Accepted: 5 September 2017 / Published: 12 October 2017

The redox flow battery (RFB), which is famous for its low cost and durability, could improve the utilization of renewable energy. We employed density functional calculations to calculate the intrinsic solubility of 9,10-anthraquinone derivatives and found that –OH groups could theoretically improve the solubility to exceed 5 mol L⁻¹. Moreover, the reduction potential was calculated for 9,10-anthraquinone derivatives with –OH substitutions at different positions. 1,8-dihydroxyanthraquinone was found to exhibit excellent electrochemical activity, as validated by electrochemical measurements. The diffusion coefficient and kinetic rate constant were faster than those of conventional materials. This is a comparatively integral work that uses first principles calculations to efficiently determine the organic redox flow of battery materials.

Keywords: Redox flow battery, First principles calculation, Solubility, Reduction potential, Anthraquinone derivatives

[FULL TEXT](#)

© 2017 The Authors. Published by ESG (www.electrochemsci.org). This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution license (<http://creativecommons.org/licenses/by/4.0/>).