

Theory-based Analysis of 1,4-Polyanthraquinone as Cathode Material for Post-Lithium Batteries

Laura Femmer^{1,2}, Lukas Köbbing^{1,2}, Juliane Heitkämper^{1,2},
Piotr de Silva³, Juan M. García-Lastra³, Birger Horstmann^{1,2,4}

¹ Institute of Engineering Thermodynamics, German Aerospace Center,
Wilhelm-Runge-Straße 10, 89081 Ulm, Germany

² Helmholtz Institute Ulm, Helmholtzstraße 11, 89081 Ulm, Germany

³ Department of Energy Conversion and Storage, Technical University of Denmark,
Anker Engelunds Vej 301, Kongens Lyngby, Copenhagen 2800, Denmark

⁴ Institute of Electrochemistry, Ulm University, Albert-Einstein-Allee 47, 89081 Ulm, Germany
laura.femmer@dlr.de

Organic materials are a promising cathode material because of sustainability, abundance, and low cost [1]. 1,4-Polyanthraquinone (PAQ) is one possible candidate that has been used for example by Z. Zhao-Karger et al. [2]. We have investigated the material by using a theory-based approach through quantum mechanical methods like density functional theory (DFT). Our aim was gaining insights into its structure and improving our understanding of its bonding properties with different metal ions used as the anode materials.

We have generated energetically comparable conformers of the PAQ-polymer with various numbers of anthraquinone units in the unit cell for periodic DFT calculations. In order to achieve this, we developed a computationally efficient approach to generate these conformers without rotational or symmetrical duplicates. To investigate the bonding of the polymer to Calcium, Magnesium, Sodium and Lithium we inserted these ions individually into these conformers and compared their energies and structures to uncover different performance capabilities experimentally observed based on the atomistic behavior.

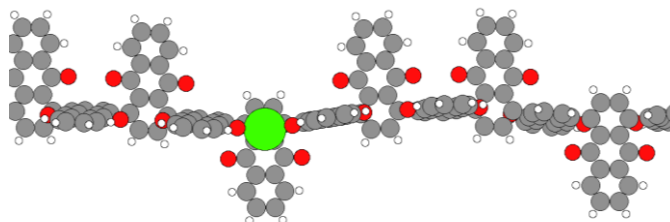


Figure: One PAQ conformer with one Calcium atom [Generated with 3, 4].

[1] J. Shea et al., ACS Applied Materials & Interfaces 12 (2020), 5361-5380.

[2] Z. Zhao-Karger et al., Nat Commun 13 (2022), 3849.

[3] A. Larsen et al., J. Phys.: Condens. Matter 29 (2017), 273002.

[4] AMS 2024.101, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, Netherlands,
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