

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

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Abstract

There is a variety of possible organic cathode materials for post-lithium batteries. One promising candidate is 1,4-polyanthraquinone (PAQ), as suggested for example by Z. Zhao-Karger et al. [1]. Our research focuses on theory-based analysis of the material, by using density functional theory (DFT) methods to gain insights into its structure, and improve our understanding of its bonding properties with different metal ions used as anode materials.

For periodic DFT calculations, we considered different numbers of anthraquinone units in the unit cell of the polymer and searched for energetically comparable conformers. To achieve this, we developed a computationally efficient approach to generate these conformers for various numbers of anthraquinones in the unit cell, ensuring that no duplicates were created through symmetry or rotation. We then inserted different metal ions into these conformers and compared their energies and structures to unveil different performance capabilities of various post-lithium ions based on the atomistic behavior.

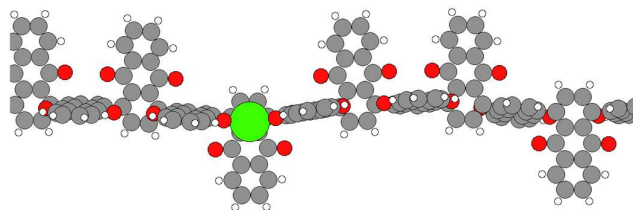


Figure: One PAQ conformer with one Calcium atom [Generated with 2, 3]

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

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

[3] AMS 2024.101, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, Netherlands, www.scm.com.

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