# Computational Study of Organic Electrode Materials

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Organic electrode materials are emerging as promising alternatives to conventional inorganic electrodes [1], offering the advantage of deminishing scarce natural resources such as cobalt and leveraging sustainable and naturally abundant chemical elements (C,N,O,S,H). Identifying and screening suitable organic materials remains a significant challenge due to their diverse structural possibilities. Atomistic simulations, often Density Functional Theory (DFT), can help to discover this huge structural space with tunable properties and unreveil structure-property relationships, allowing for rational design of improved organic electrode materials.

1,4 Polyanthraquinone (PAQ) is one relevant example that has been explored in post lithium battery concepts [2]. A quantum mechanical framework is employed for the investigation and rational design of such organic electrode materials. Density functional theory (DFT) is used to explore the PAQ polymer via a workflow that efficiently generates energetically comparable conformers with varying numbers of anthraquinone units in the periodic unit cell and enables the analysis of structure-bonding relationships in the presence of Li, Na, Ca, and Mg ions. This provides atomistic insight into ion specific coordination, structural stabilization, and trends that help rationalize experimentally observed performance differences [5].

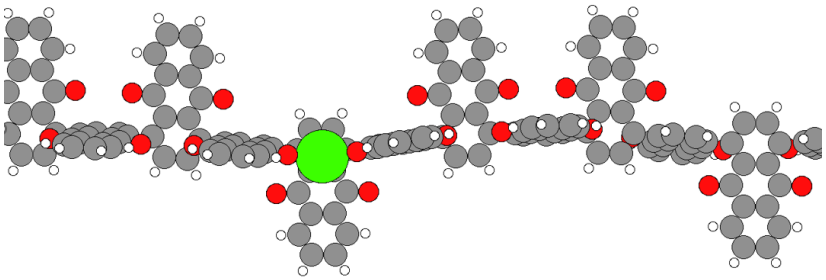

Figure 1: One PAQ conformer with one Calcium atom (Generated with [3, 4]).

## References

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