Tunable organic polymers for Na-aqueous batteries

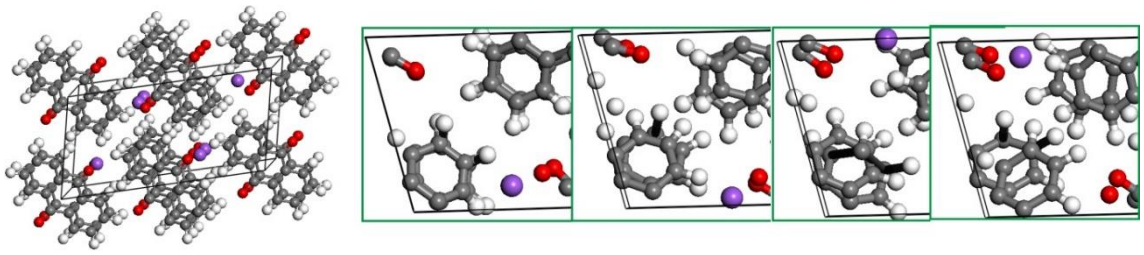
Remco van der Jagt [a], Alexandros Vasileiadis [a], Wolter F. Jager [b], Kajan Kort [a], Marnix Wagemaker [a]

[a] *Storage of Electrochemical Energy (SEE), Department of Radiation Science and Technology, Faculty of Applied Sciences, Delft University of Technology, Mekelweg 15, 2629 JB Delft, The Netherlands*

[b] *Organic Materials & Interfaces (OMI), Department of Chemical Engineering, Faculty of Applied Sciences, Delft University of Technology, Van Der Maasweg 9, 2629 HZ Delft, The Netherlands*

E-mail: *R.vanderJagt*@tudelft.nl

The lack of low-cost well performing anode materials for Na-aqueous battery prevents its real breakthrough, whereas it appears to be a promising solution for the energy storage challenge. Tremendous amounts of cost-effective stationary energy storage is required to maintain a constant supply of renewable electricity. Organic materials are very promising battery candidates, since they consist of abundant elements, have tunable properties, are flexible and can easily be produced at a mass scale [1]-[3]. The instability of organic materials appears to be one of the remaining thresholds to overcome. Polymerization of organic materials seems to be an effective solution for this. However, common polymerization techniques, e.g. imidization or sulfurization, are rather uncontrollable techniques since they proceed too fast and are too spontaneous. This results in clustered polymers with rigid structures which are (too) hard for electrode processing. In the presented work, multiple carbonyl-based organic battery materials (e.g. the anhydride and quinone family), were identified by performing DFT-calculations. DFT enabled the determination of binding energies and enthalpies of formation revealing the relative phase stability and giving insight regarding the reaction mechanisms. The kinetic performance in organic frameworks was studied via Molecular Dynamic (MD) simulations, providing a clear picture regarding power capability. Following the initial computational screening that involved evaluation of fundamental thermodynamic, structural and kinetic properties, novel organic electrodes were synthesized and characterized (XRD, IR and NMR). These materials were selected to withstand multiple criteria e.g. appropriate working potentials, electrochemical stability and small volume change upon sodiation. Attachment of electron donating or withdrawing groups to the materials have also been investigated for tuning the electrode potentials to the desired value. Furthermore, a new two steps facile and controllable polymerization method has been introduced to obtain flexible battery materials, which is also preferable for battery processing at large scale.



References:

[1] Z. Song, H. Zhou, Energy & Environ. Sc., 2013, **6**, 2280-2301.

[2] Y. Liang, Z. Tao, J. Chen, Adv. Energy Mat. 2012, **2**, 742-769.

[3] B. Häupler, A. Wild, U.S. Schubert, Adv. Energy Mat. 2015, **5**, 1402034.