Molecular modelling of hybrid-ion batteries

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Batteries have been a constant target of research and improvement but the competition in this field has never been as strong as nowadays. All sorts of devices rely on them starting from pacemakers and hearing aids through mobile electronic devices and electric cars to stations for storage and redistribution of energy obtained from renewable sources or excess energy from power plants. Therefore, any effort to enhance their performance is welcome.

There exist numerous types of batteries but those that have undergone the fastest progress in the past decades are the lithium-ion batteries. However, their demand is high, their price remains steep and the deposits of lithium are depleting. An attractive alternative pricewise are the sodium-ion batteries but they are less efficient for mobile applications. Therefore, hybrid-ion batteries could be a solution but it requires extensive research and design of all components: electrodes and electrolyte solutions.

The traditional electrode materials are of inorganic origin. Their replacement with organic ones will reduce the cost and the weight, will be flexible and, hopefully, will improve the performance. In the present, based on doped or functionalised carbonaceous materials are modelled by means of first principles methods and the type of interaction with some light metal ions is discussed. The non-aqueous solvents should provide the efficient mobility of the charge carriers. The electrolyte-solvent interplay is discussed in terms of coordination number of the ions, of the free energy of their solvation/desolvation, and of the competition between the solvated ions. The cations considered are Li^+, Na^+, and Mg^{2+} (neutralized by PF_6^-) and the solvent is ethylene carbonate.

The outcomes can serve as guidelines for enhancement of the performance of hybrid-ion batteries.

Acknowledgments: The research was supported by projects D09/13/2016, and the National Research Program E+, grant D01-214/28.11.2018. The Erasmus+ internship program and the mentorship of Prof. Patrik Johansson's group at Chalmers University of Technology is acknowledged.