Towards efficient electrolytes for Ca batteries: A COSMO-RS approach

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Multi-valent ion based battery chemistries such as Mg, Ca and Al batteries have recently (re-)emerged as alternatives to the prevalent Li-ion batteries. Here we highlight the advantages of Ca as compared to Mg and Al: abundant in the Earth's crust – hence sustainable, lower standard potential – hence enabling cells of higher voltage, and a "softer" cation – with a possibility of faster cation diffusion, especially in the solid state.

There are, however, still numerous challenges to overcome to create a functional Ca battery, one central being to develop a Ca conducting electrolyte enabling reversible Ca plating and stripping *vs*. Ca metal negative electrodes at room temperature. Here we outline the framework of using a fluid-phase thermodynamics approach, the conductor-like screening model for real solvents (COSMO-RS) [1, 2], to screen for Ca battery electrolytes. This approach has recently been proven effective in the development of novel Li-S battery electrolytes, both to estimate the solubility of sulfur [3] and deciphering the real advantages of applying fluorinated solvents [4]. A large number of Ca battery electrolyte materials and compositions have been investigated using an array of key performance indicators to guide subsequent physico-chemical and electrochemical tests.

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