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Materials for Li & Na Batteries : A Computational Materials Science Point of View

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Energy storage has been a theme for scientists for two hundred years. The Lead acid battery research on batteries occupied some of the best minds of the 19th century. Gaston Plante in 1859 invented the lead acid battery which starts your car and ignites the internal combustion which takes over the propulsion. Although the lead battery is over 150 years old but the origin of its open circuit voltage (OCV) of 2.1 V is still known. In present talk, I will show how one can explain the origin of OCV of 2.1 V based on foundations of relativistic quantum mechanics. Surprisingly, seems to be the first time its chemistry has been theoretically modeled from the first principles of quantum mechanics. The main message of this work is that most of the electromotoric force (1.7-1.8 Volts out of 2.1 V) of the common lead battery comes from relativistic effects. While the importance of relativistic effects in heavy-element chemistry is well-known since over two decades, this is a striking example on "everyday relativity". We believe that the fact that "cars start due to relativity."

The purpose of this talk is to provide an overview of the most recent theoretical studies undertaken by us in the field of materials for Li & Na ion battery research. For selected examples, I will show how ab initio calculations can be of use in the effort to reach a better understanding of battery materials and to occasionally also guide the search for new promising approaches. Systems to be discussed include : Li2FeSiO4, Na2FePO4F, transition-metal-doped NiTiH hydrides, Na air batteries etc.