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Beller Lectureship: 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 19th century. Plante in 1859 invented lead acid battery which starts your car and ignites 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. The main message of this work is that most of the electro-motoric force of the common lead battery comes from relativistic effects. In second part, I will provide an overview of the most recent theoretical studies undertaken by us in the field of materials for Li & Na ion batteries. 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 materials.