Abstract Submitted
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First-principles study of the electronic properties and discharge profile of $AgNa(VO_2F_2)_2$[1] MASATOSHI ONOUE, GIANCARLO TRIMARCHI, ARTHUR J. FREEMAN, Northwestern U., Evanston (IL) — Implantable cardiac defibrillators (ICDs) require batteries with high capacities and high discharge rates to ensure the optimal operation of the device over several years. $Ag_2V_4O_{11}$ has been a cathode material of choice for the ICDs owing to its high capacity and fast rate of electronic discharge. To reduce ICD size and improve ICD performance, a new cathode material would need to display a higher volumetric capacity and redox potential. Recently, the new cathode compound $AgNa(VO_2F_2)_2$ (SSVOF) was synthesized and displayed favorable voltage for sodium-ion batteries. However, the discharge reaction has been unclear. In this presentation, we study the discharge reaction of SSVOF through DFT calculations. All calculations are performed within the PAW method using the GGA and GGA+U functionals. Among several possible reactions, we focus on the reaction $AgX + A \rightarrow AX + Ag$, where X is $Na(VO_2F_2)_2$ and A is Li or Na. In this reaction, the discharge occurs by replacing Ag with A. The calculated discharge potential for Li is 3.3 V in GGA and 2.9 V in GGA+U and that for Na is 3.1 V in GGA and 2.8 V in GGA+U. These values are consistent with the experimental ones.

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