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## DFT study of AlF<sub>3</sub> intercalated in HOPG: a rechargeable battery application

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Currently, rechargeable ion batteries are attracting more attention than others due to their advantages as recycling charging devices with high energy capacity, high performance, and easy adaptation to industry [1,2]. Lithium-ion batteries (LIBs) are currently the best performing batteries mainly due to their relatively high energy densities, good stability, and low self-discharge. Their main deficiencies are the limited resources of lithium and the poor distribution of its raw materials throughout the world [3]. This concern has prompted research into alternative systems based on different types of metal-ion batteries, such as aluminum (Al), sodium (Na), magnesium (Mg), and Zinc (Zn), whose applications range from personal electronics to grid storage. Batteries employing metallic Al as the anode material show considerable promise due to their low cost, ease of handling under ambient conditions, and high theoretical capacities (with energy densities of 30-70 Wh kg<sup>-1</sup>). On the other hand, graphite is the material mostly used as a cathode in ion batteries, mainly due to its ability to capture ions, atoms, or molecules inside [4]. Several theoretical and experimental studies have focused on the appropriate combination of host species and graphite cathodes to improve the recharging performance of aluminum batteries. In this talk, a theoretical study in the density functional theory (DFT) formalism is reported to explain surface intercalation experiments of neutral AlF<sub>3</sub> on highly oriented pyrolytic graphite (HOPG) [5,6].

### References

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