Theoretical Studies of Charge Transport in Rechargeable Batteries:
Lithium-ion and Metal-air Batteries

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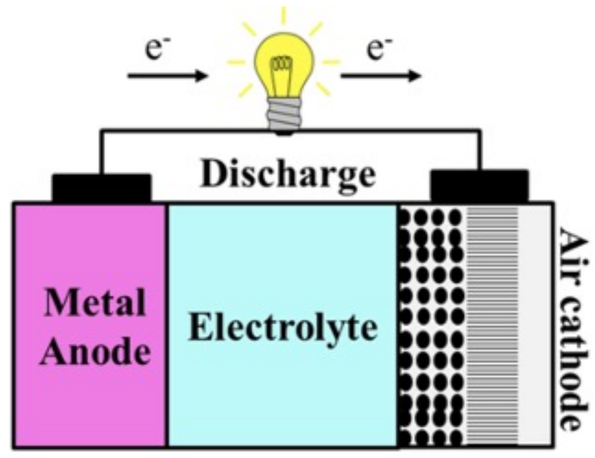
Introduction

Today, most electric vehicles and hybrid electric vehicles rely on Li-ion batteries. The main drawbacks of Li-ion batteries are their high price, slow charging, and low energy/power density compared with that gasoline. In the past two decades, significant efforts have been paid to the development of metal–air batteries (e.g., Li–, Na–, Mg–, Al– and Zn–O_2). They are promising in the making of economical and efficient batteries in the transport sector. But, there are several shortcomings that hinder the practicality such as poor conductivity and rechargeability, dendrite, H_2O and CO_2 contamination, and stability of electrodes and electrolytes.



Computational Methods

✓ We employed DFT implemented in the GPAW code

GPAW!

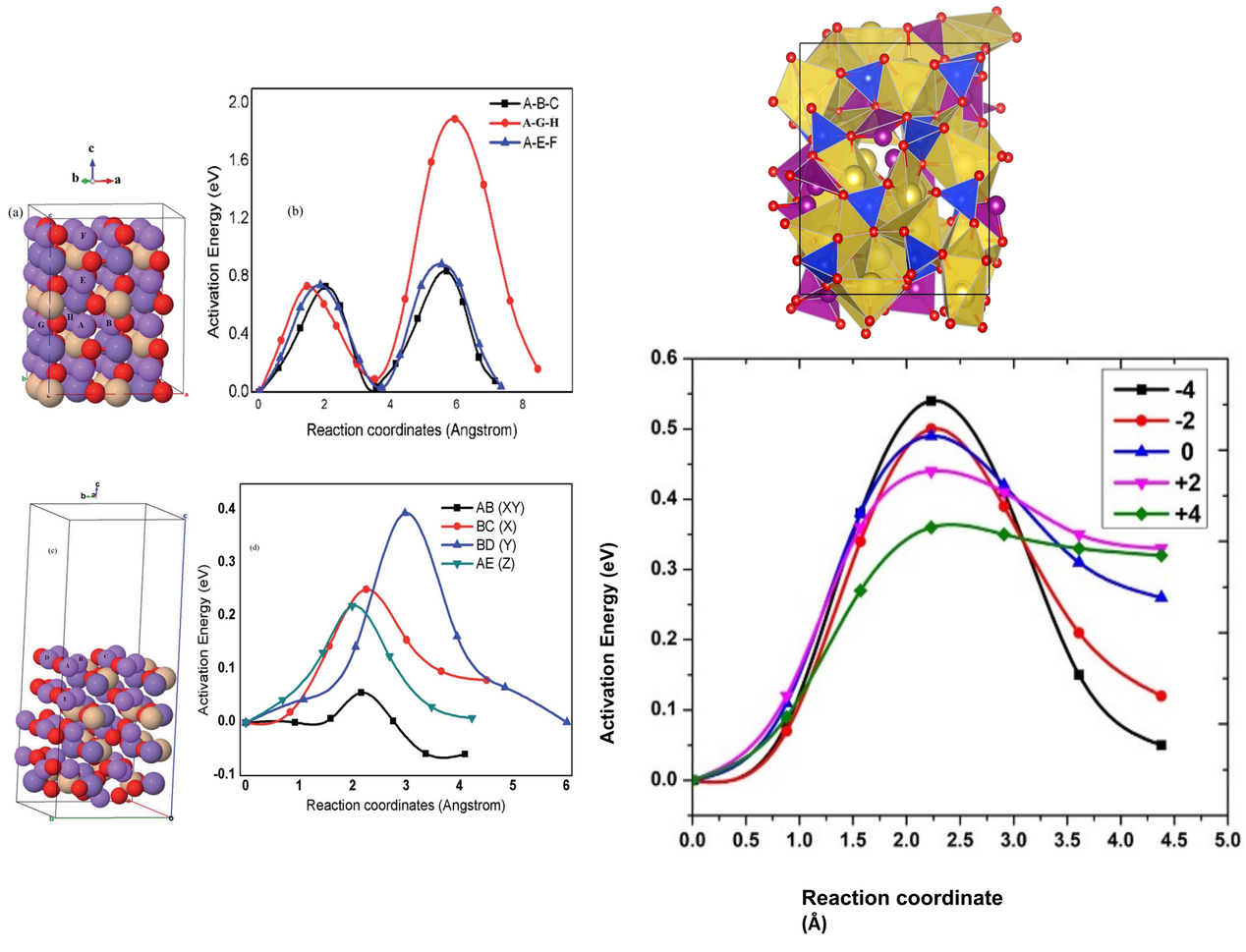
Results and discussion

- ✓ DFT + U (at U=3 eV) results indicated that the bulk Li_2MnSiO_4 is an insulator (3.42 eV) whereas the (001) surface is nearly metallic with a bandgap of 0.6 eV.
- ✓ Li vacancies found to be prone to trapping at the peroxide part of the interface
- ✓ During discharge, Li_2O_2@Li_2CO_3 interfaces provide an alternative in-plane channel for fast electron polaron hopping
- ✓ NaO2@Na2CO3 interface exhibited the lowest bandgap, implying half metallic character and thus improving the electronic properties.

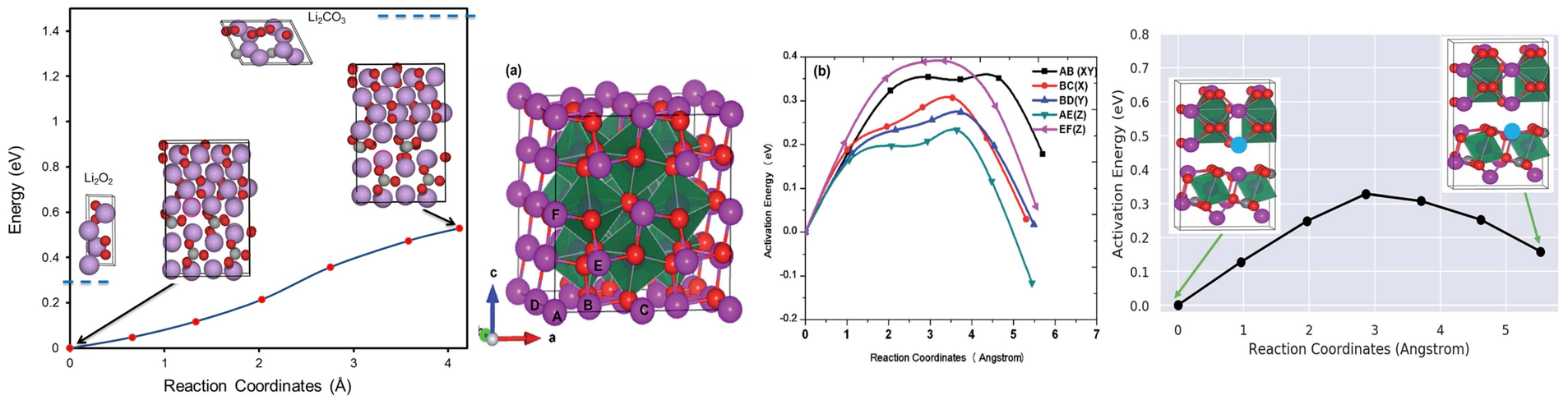
Conclusion

- ✓ The (001) Li_2MnSiO_4 revealed fast ionic diffusion in all 3D with over 12-orders-of- magnitude compared with the bulk system. Moreover, the biaxial strain studies also revealed an improved the conductivity in Na_2MnSiO_4.
- ✓ Despite the insulating nature of discharge products (Li_2O_2, NaO_2, Na_2O_2, Na_2CO_3, and the cathode-electrolyte interfaces) of metal-air batteries, Li^+ and Na^+ -ions diffusions at a high rate with an energy barrier of < 0.5 eV.
- ✓ Charge transport studies showed that surfaces and interfaces offer an improved ionic and electronic conductivity.

Li^+ and Na^+ ion diffusion in Lithium–ion batteries



Li^+ and Na^+ ion diffusion in Metal–air batteries



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