Computational Study of Interfacial Phenomena for Battery Applications

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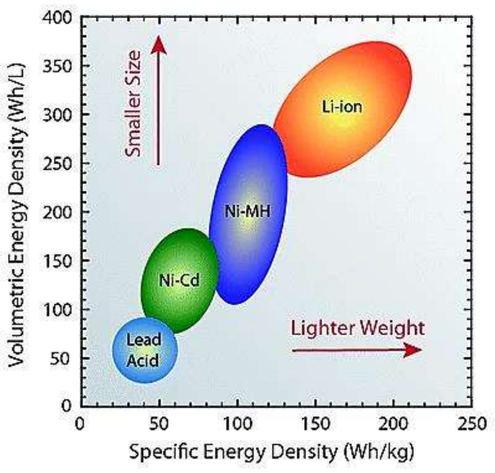
Background

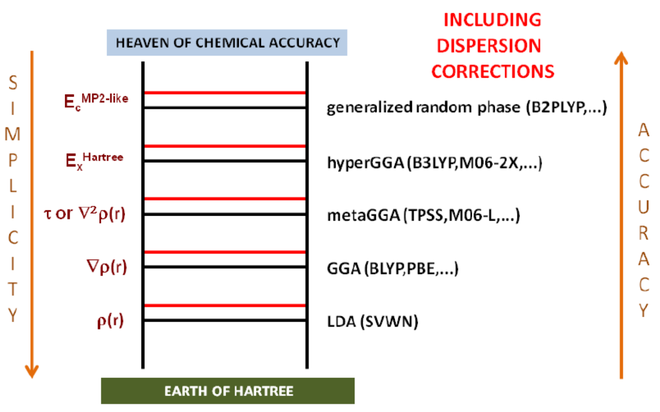


Retrieved from
http://www.epectec.com/batteries/cell-comparison.html

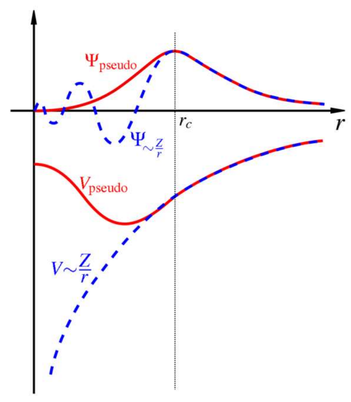
- **We need cheaper and safer batteries with high energy density.**
- ***Ab-initio* modeling guides materials design.**

Methodology

- **Density Functional Theory (DFT) used to compute the electronic structure of matter. Implemented using the VASP package.**



Gomes, J.; Fajín, J. L.; Cordeiro, N.; Teixeira, C.; Gomes, P.; S. Pillai, R.; Novell-Leruth, G.; Toda, J.; Jorge, M., *Density functional treatment of interactions and chemical reactions at surfaces*. 2013; p Density functional treatment of interactions and chemical reactions at surfaces.



Retrieved from
https://en.wikipedia.org/wiki/Pseudopotential

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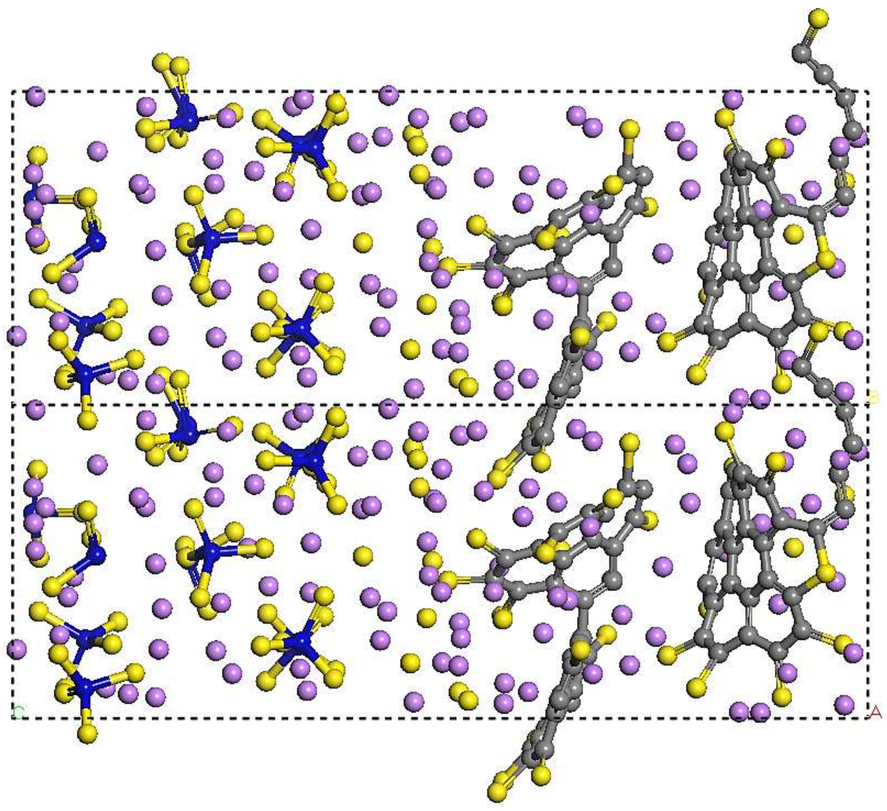
Li/S Batteries

Solid-State Electrolytes (SSE)-C/S (Cathode) Interface

P S C Li

(100) $Li_7P_3S_{11}$

C/S Cathode, Sulfur content: 61 wt %



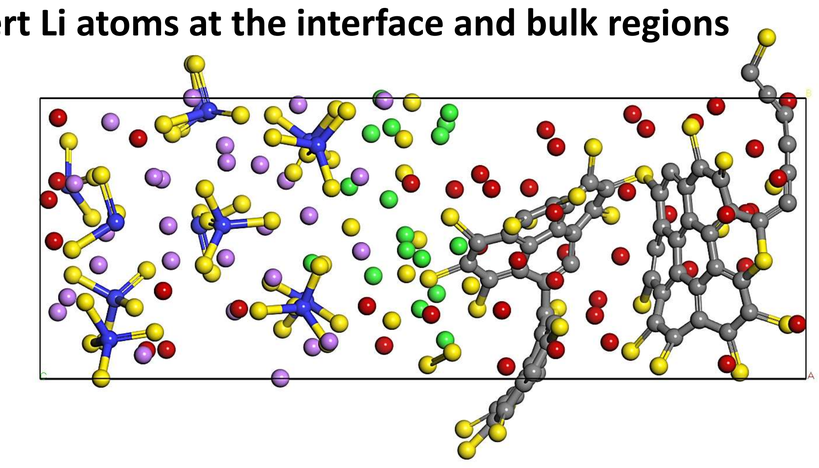
Snapshot at 28 ps

- **Interface connection formed (S-S and Li-S pairs)**

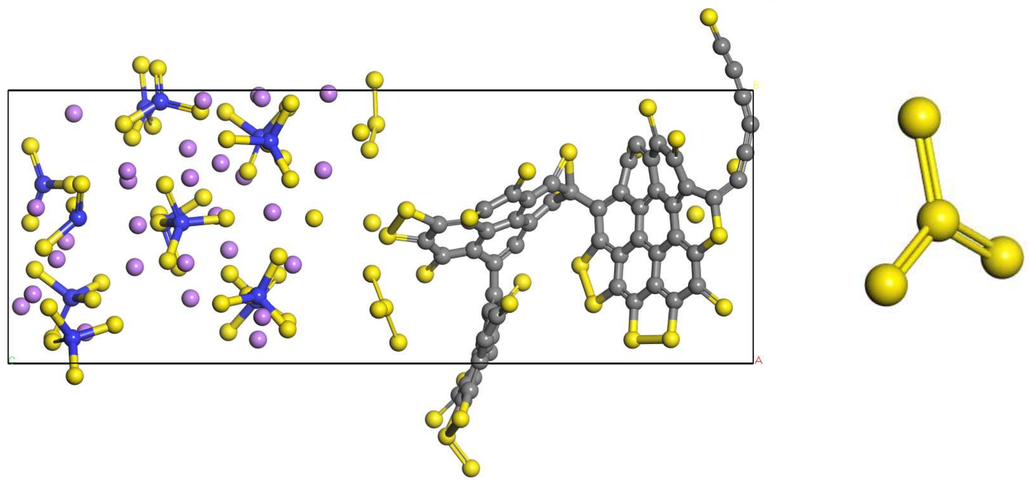
Li/S Batteries (Cont'd)

Simulated Charge Analysis

1- Insert Li atoms at the interface and bulk regions



2- Remove Li atoms at the interface and bulk regions

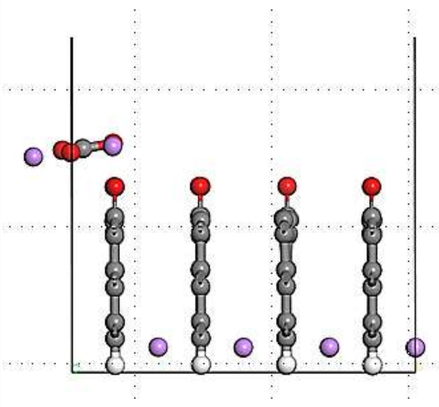


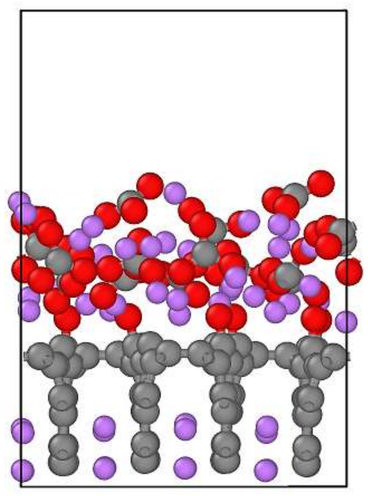
- **S_3 and S_4 formation at the interface**

Li-Graphite System

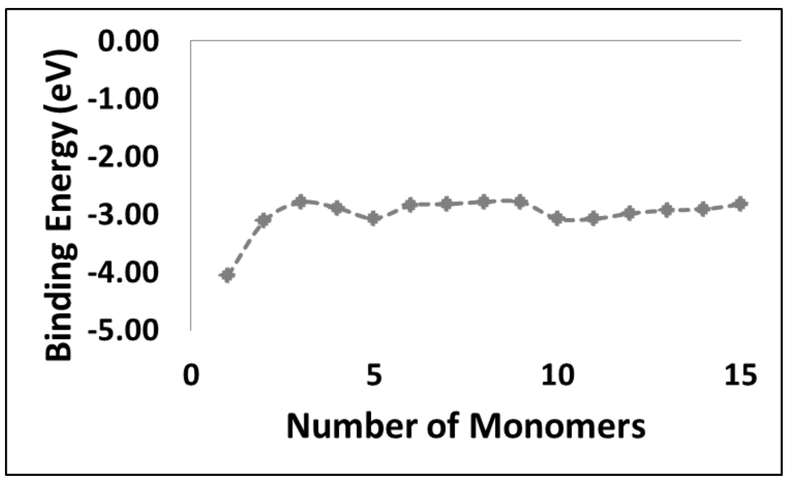
Electrode-Electrolyte Interface

C O Li





$$Ebind = \frac{\text{Etotal} - \left(\text{Eanode} + (\text{n} * \text{Emonomer})\right)}{n}$$



- Li_2CO_3 strongly adsorbed at the surface
- Li_2CO_3 block formed on top of the lithiated graphite slab

Conclusions

- **With the help of high-performance computer clusters, ab-initio modeling is used to gather information and knowledge of molecular events.**
- **This knowledge is used to guide the design of next-generation materials.**

Computation performed on
Texas A&M High Performance Research Computing
Ada and Terra Clusters

b-initio VASP ackage imulation ienna

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