Theoretical study of the interface between solid electrolyte and electrode: the case of (100)-Li_3PS_4/(110)-Li_2S

Naiara L. Marana[1,*], Silvia Casassa[1], Mauro F. Sgroi[2], Anna Ferrari[1], and Lorenzo Maschio[1]

[1]Theoretical Group of Chemistry, Chemistry Department I.F.M., Torino University, Italy

[2]Centro Ricerche Fiat S.C.p.A., Strada Torino 50, Orbassano, 10043, Italy

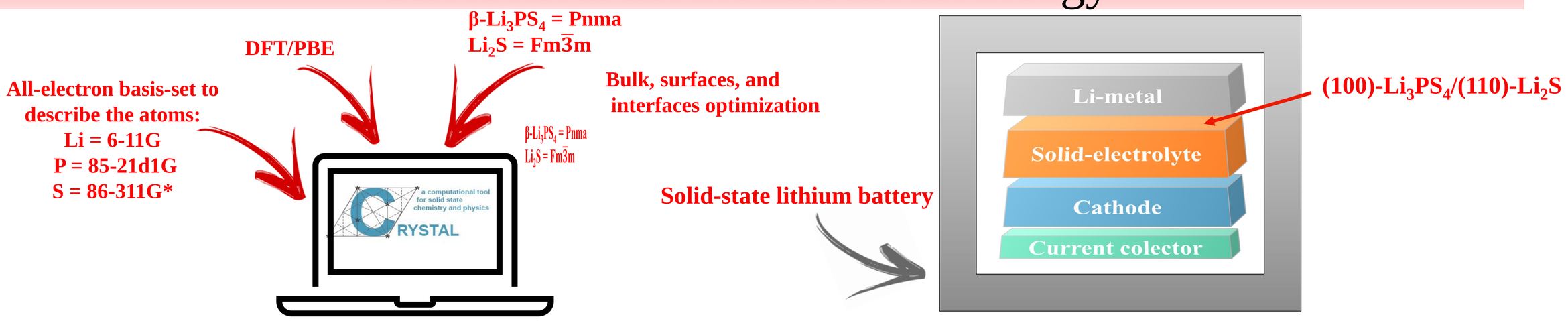
naiaraleticia.marana@unito.it

Introduction

With the considerable reduction of fossil fuels and the growing search for renewable and inexhaustible energies, research in the area of batteries has increased in recent decades. In this context, lithium-ion batteries emerged, which are efficient, light, and safe, with good energy storage and good stability. Widely used in small devices such as cell phones, it has also been studied for use in electric cars. However, many problems still need to be solved for such batteries to become safe, efficient, and marketable, such as the implementation of solid electrolytes and their compatibility with battery electrodes. MODALIS² is a transnational European research program that aims at investigating new materials for next-generation lithium-ion batteries for electric vehicles.

Supported by MODALIS², this study aimed to investigate theoretically, through DFT the interface between the solid-state electrolyte β-Li_3PS_4 and the passivating material Li_2S, to analyze their compatibility.

Theoretical model and methodology



Results

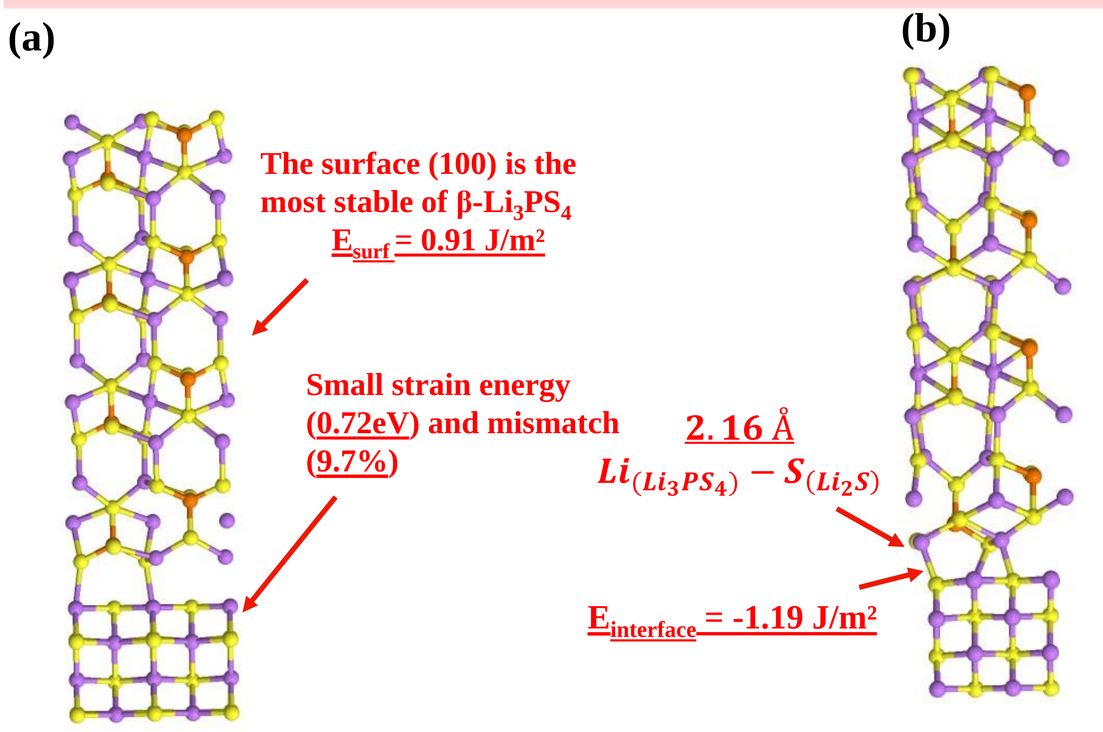


Figure 1: Interface of the (a) initial models and (b) optimized interface (100)-Li_3PS_4/(110)-Li_2S

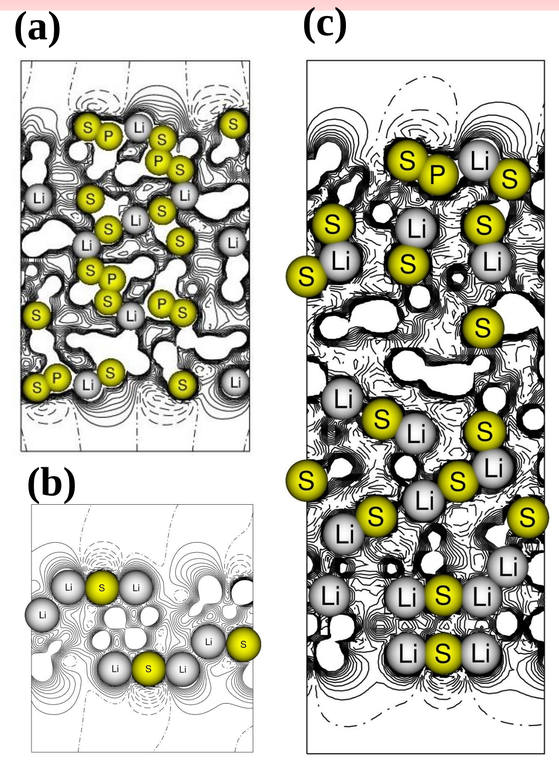


Figure 2: Electrostatic Potential maps of the initial models (a) (100)-Li_3PS_4 and (b) Li_2S and (c) optimized interface (100)-Li_3PS_4/(110)-Li_2S

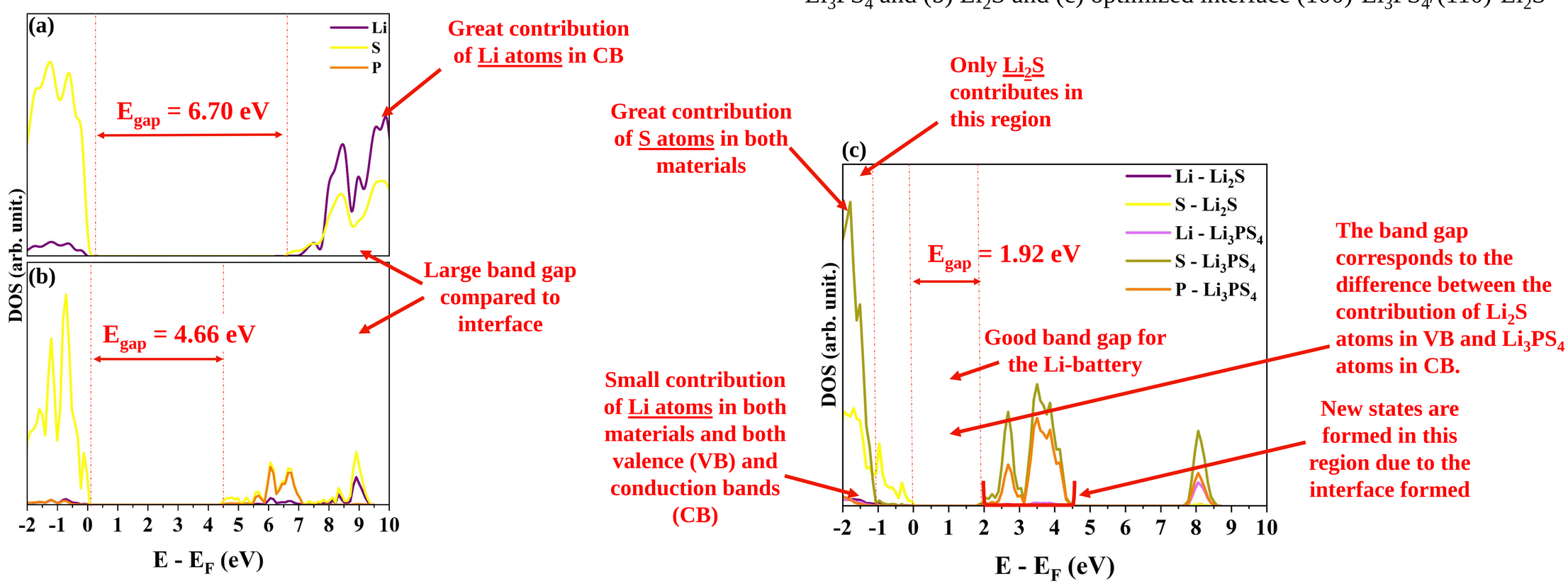


Figure 3: Projected-DOS of isolate systems (a) Li_2S and (b) (100)-Li_3PS_4, and of the optimized interface (100)-Li_3PS_4/(110)-Li_2S

Acknowledgmets

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References

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