Title : Analysis of Si surface/polymers interface for self-healed next generation Lithium ion batteries

Silicon anode suffers from poor intrinsic conductivity and dramatic volume change during discharge/charge process[1, 2], which hinders its commercialization for high energy density lithium-ion batteries(LiBs). This issue can be alleviated by embedding particles of the active material in an adhesive matrix, such as a polymer binder [3], that can accommodate large volume changes during lithiation and delithiation. Several research efforts have aimed at enhancing the adhesive, elastic, electrical, and ionic properties of binders for use in Si anodes [1, 3, 4, 5]. Therefore stable silicon/polymer interfaces[6] are crucial for the performance of high capacity of silicon based LiBs. In particular we will focus on silicon and new self-healing polymers as new promising anode material for next-generation high-energy-density LiBs.

In this presentation from first-principles calculation based on density functional theory (DFT), some initial challenges of self-healing properties of polymeric binders, B-doped polyaniline (PANI)/ polyvinylalcohol (PVA) polymers have been explored. To simulate the effect that different functionalizing molecules can have on the electronic/mechanical properties of a Si based anode surface, we started with:
1) different silicon surfaces and their possible reconstructions,
2) different anchoring geometry of the binders on the surfaces before and after lithiation.

In this presenetation I will discuss functionalization of Si(110) suraface with B-doped polyaniline (PANI)/ polyvinylalcohol (PVA) followed by lithiation of the surface. The structural evolution and corresponding electronic properties as a function of Li concentration will be discussed.

References:
1. S. Huang et al. Int. J. Energy Res. 2018, 42, 919−935
2. M. N. Obrovac et al. Electrochem. Solid-State Lett. 2004, 7, A93−A96.
3. Manav Bhati and Thomas P. Senftle J. Phys. Chem. C 2019, 123, 27036−27047
4. T.-w. Kwon et al. , Chem. Soc. Rev. 2018, 47, 2145−2164
5. Q. Y. Zhang et al. , Adv. Sci. 2020, 7, 2000749
6. Andrea Miranda et al. , Mol. Syst. Des. Eng., 2020, 5, 709

Authors :
Rita Maji
Dipartimento di Scienze e Metodi dell'Ingegneria, Università di Modena e Reggio Emilia, Via Amendola 2 Padiglione Tamburini, I-42122 Reggio Emilia, Italy
Michele Aparecida Salvador
Dipartimento di Scienze Fisiche, Informatiche e Matematiche sede ex-Fisica, Università di Modena e Reggio Emilia,Via Campi 213/A, 41125 Modena
Elena Degoli
Dipartimento di Scienze e Metodi dell'Ingegneria, Università di Modena e Reggio Emilia, Via Amendola 2 Padiglione Morselli, I-42122 Reggio Emilia, Italy
Centro Interdipartimentale En&Tech, Via Amendola 2 Padiglione Morselli, I-42122 Reggio Emilia, Italy
Centro S3, Istituto Nanoscienze-Consiglio Nazionale delle Ricerche (CNR-NANO), Via Campi 213/A, 41125 Modena, Italy

Alice Ruini , Rita Magri
Dipartimento di Scienze Fisiche, Informatiche e Matematiche sede ex-Fisica, Università di Modena e Reggio Emilia,Via Campi 213/A, 41125 Modena