Modeling self-healing binders for silicon anodes

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Silicon anodes typically suffer from poor intrinsic conductivity and dramatic volume change during charge/discharge cycles, leading to surface cracks and, eventually, to anode pulverization. A promising way to overcome these failures is to embed the silicon particles in a conductive self-healing binder. In the EU project Bat4ever, autonomous self-healing is introduced through silicon polymer-coated particles to be implemented as anodes in the self-healing batteries. Atomistic first-principles and molecular dynamics simulations have been carried out to study self-healing B-OH-PANI and PVA monomers and dimers and their interaction with silicon surfaces. We have derived the lowest energy configurations of the monomers and dimers and studied their mutual interaction, which leads to a large number of dynamic hydrogen bonds (see figure). The study of the interaction of the monomers with silicon surfaces has revealed both the formation of surface bonds and longer range electrostatic interactions. The co-adsorption of B-OH-PANI and PVA leads to a larger polymer adhesion energy relative to the adsorption of single B-OH-PANI and PVA monomers.

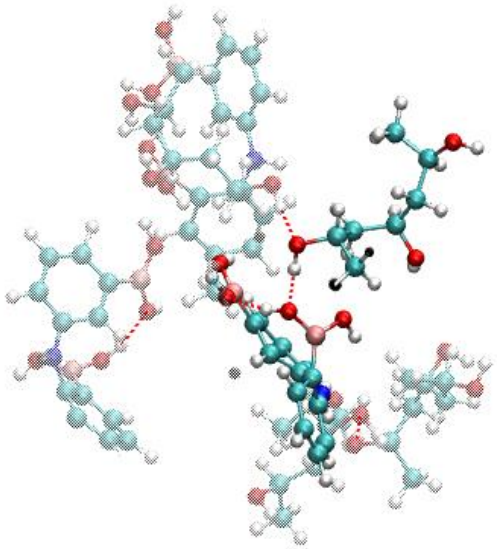

Figure 1. B-OH-PANI and PVA monomer configurations from Molecular Dynamics Simulation. The red dotted lines indicate the hydrogen bonds

REFERENCES

[1] R. Maji, M. A. Salvador, A. Ruini, R. Magri, E. Degoli, "A first-principles study of self-healing binders for next-generation Si-based lithium-ion batteries", Materials Today Chemistry 29 (2023) 101474

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