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Atomistic Insights into SEI Formation from Ionic Liquid Electrolytes on Sodium Metal: A DFT Study

Sodium batteries have attracted increasing attention as cost-effective and sustainable alternatives to lithium-ion batteries. Sodium is naturally abundant, cheaper, and operates at a lower voltage than lithium [1]. Recently, metal anode batteries have gained prominence over metal-ion systems due to their higher theoretical capacities. However, sodium metal anode batteries using conventional organic electrolytes face serious challenges, including dendrite formation and unstable solid electrolyte interphase (SEI) layers [2]. Thus, the choice of electrolyte plays a critical role in improving battery stability and performance. Ionic liquids (ILs) offer promising solutions owing to their high thermal and electrochemical stability and excellent ionic conductivity [3]. To gain atomistic insights into SEI formation and stability, we investigated the interaction of the IL [PYR13][FSI] with the Na [001] surface based on density functional theory (DFT), using the Vienna Ab-initio Simulation Package (VASP). Van der Waals dispersion-corrected DFT calculations were performed using the GGA-PBE functional and PAW pseudopotentials for both cis and trans isomers of [PYR13][FSI], considering multiple adsorption configurations on Na [001] surface. The most stable configurations exhibited adsorption energies of -1.34 eV (cis-FSI) and -1.46 eV (trans-FSI), with no decomposition of IL observed during structural optimization. Subsequent analyses examined sodium migration from the surface to the IL, followed by dissociation of the FSI anion. The migrated Na atom tends to move back to the surface exhibiting a Bader charge transfer of approximately +1 |e|, indicating Na^+ character. The $[PYR13]^+$ cation remained intact in all cases. Nudged elastic band (NEB) calculations revealed a barrierless fluorine dissociation from FSI^-. Ab initio molecular dynamics (AIMD) simulations further confirmed FSI decomposition and the formation of key SEI components, including NaF, Na2O , and Na2S. Thus, this study provides critical insights into IL-based SEI formation on sodium metal, contributing to the development of safer, high-performance sodium-metal batteries.

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