Supporting Information

Revealing the chemical compatibility of common solvents and electrolytes with Mo_2TiC_2-based MXenes and Their Interfaces in Aluminum Ion Batteries (AIBs) from First-principles Molecular Dynamics Simulations

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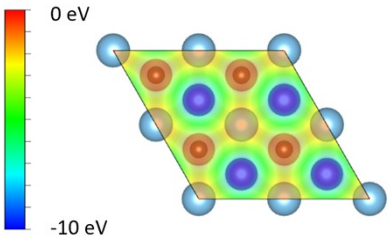

Figure S1. Electrostatic potential of Mo_2TiC_2 surface.

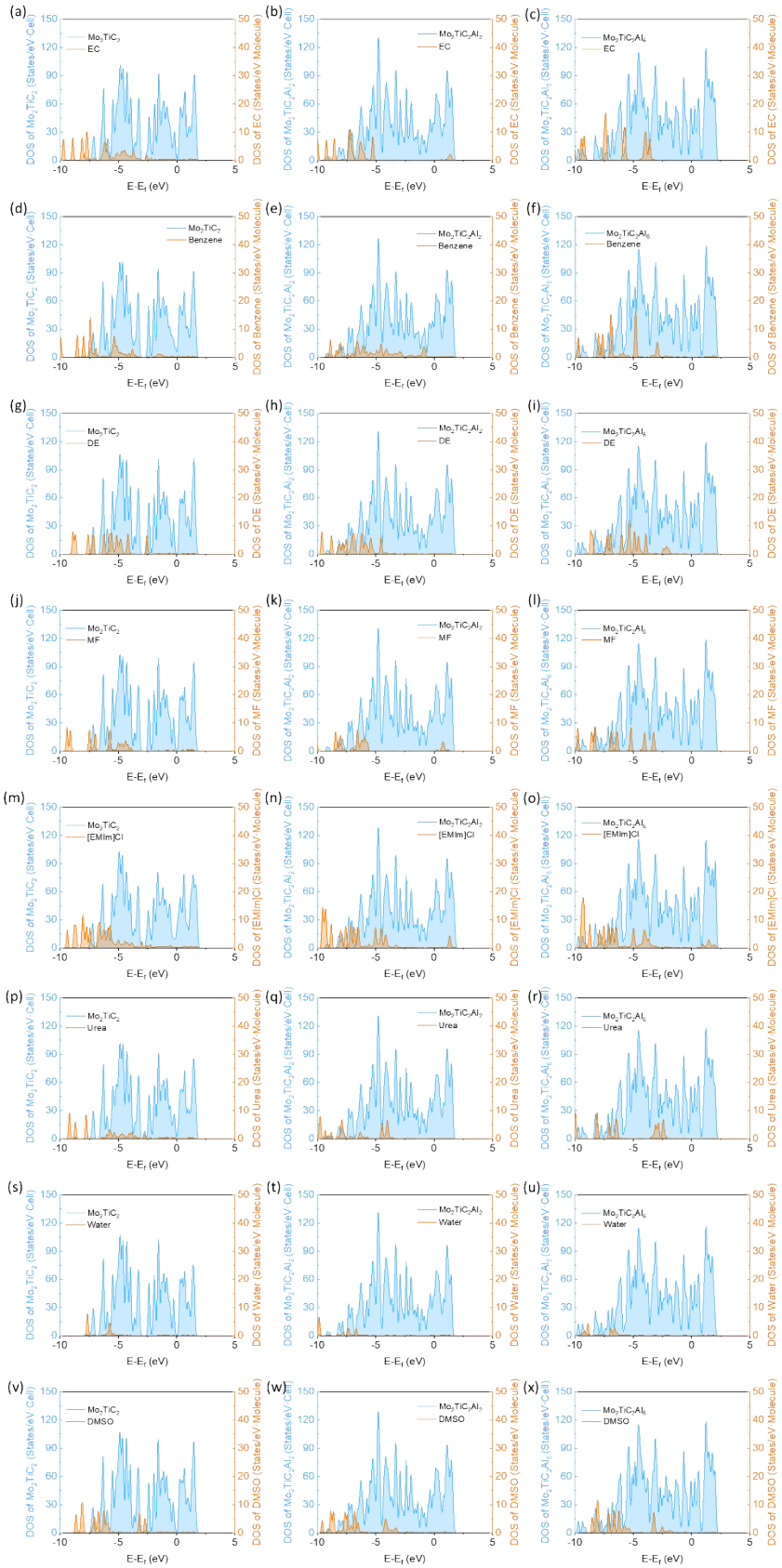

Figure S2. Electronic density of states of adsorbed molecule on Mo_2TiC_2, $Mo_2TiC_2Al_2$ and $Mo_2TiC_2Al_6$. (a)-(c) EC, (d)-(f) Benzene, (g)-(i) DE, (J)-(l) MF, (m)-(o) [EMIm]Cl, (p)-(r) urea (s)-(u) water and (v)-(x) DMSO.

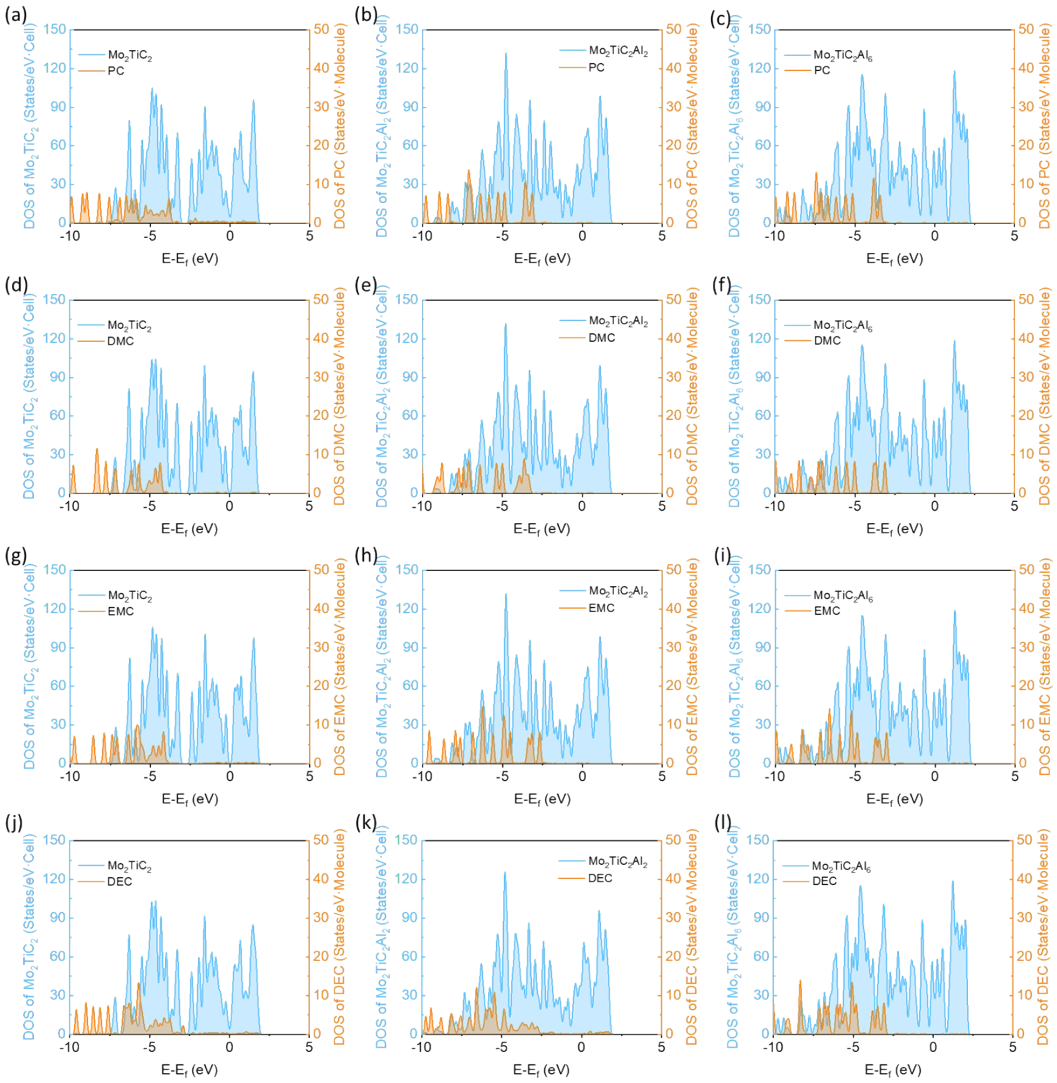

Figure S3. Electronic density of states of adsorbed molecule on Mo_2TiC_2, $Mo_2TiC_2Al_2$ and $Mo_2TiC_2Al_6$. (a)-(c) PC, (d)-(f) DMC, (g)-(i) EMC, (J)-(l) DEC.

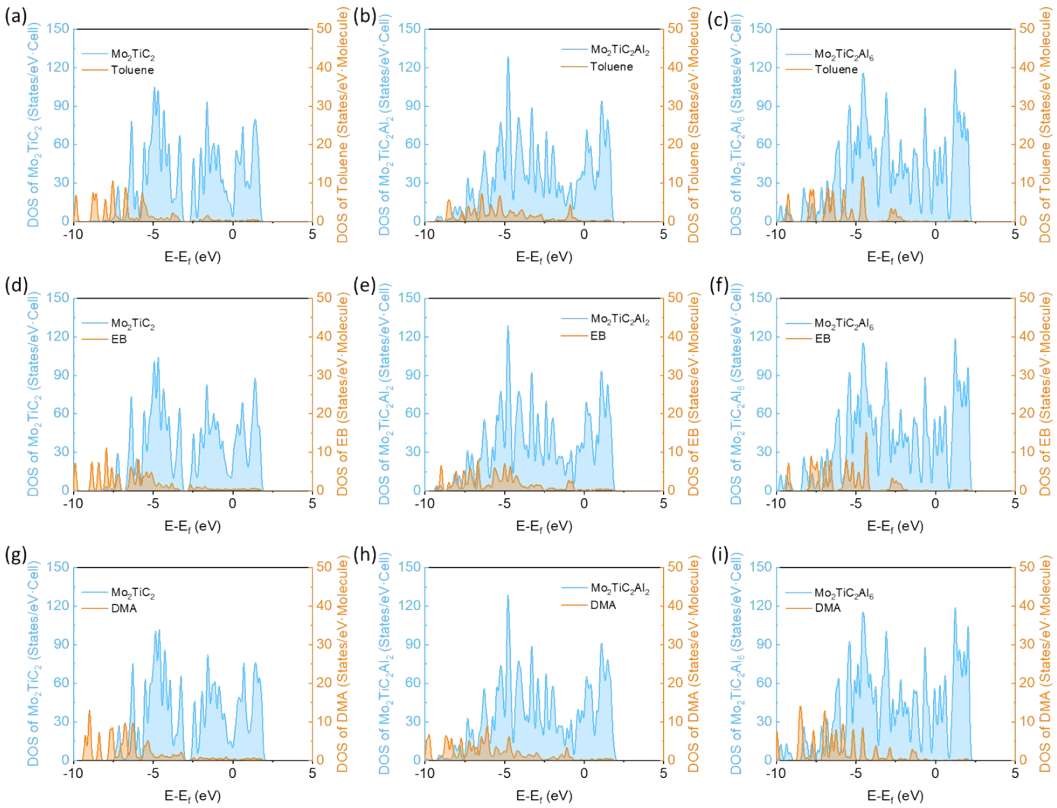

Figure S4. Electronic density of states of adsorbed molecule on Mo_2TiC_2, $Mo_2TiC_2Al_2$ and $Mo_2TiC_2Al_6$. (a)-(c) toluene, (d)-(f) EB, (g)-(i) DMA.

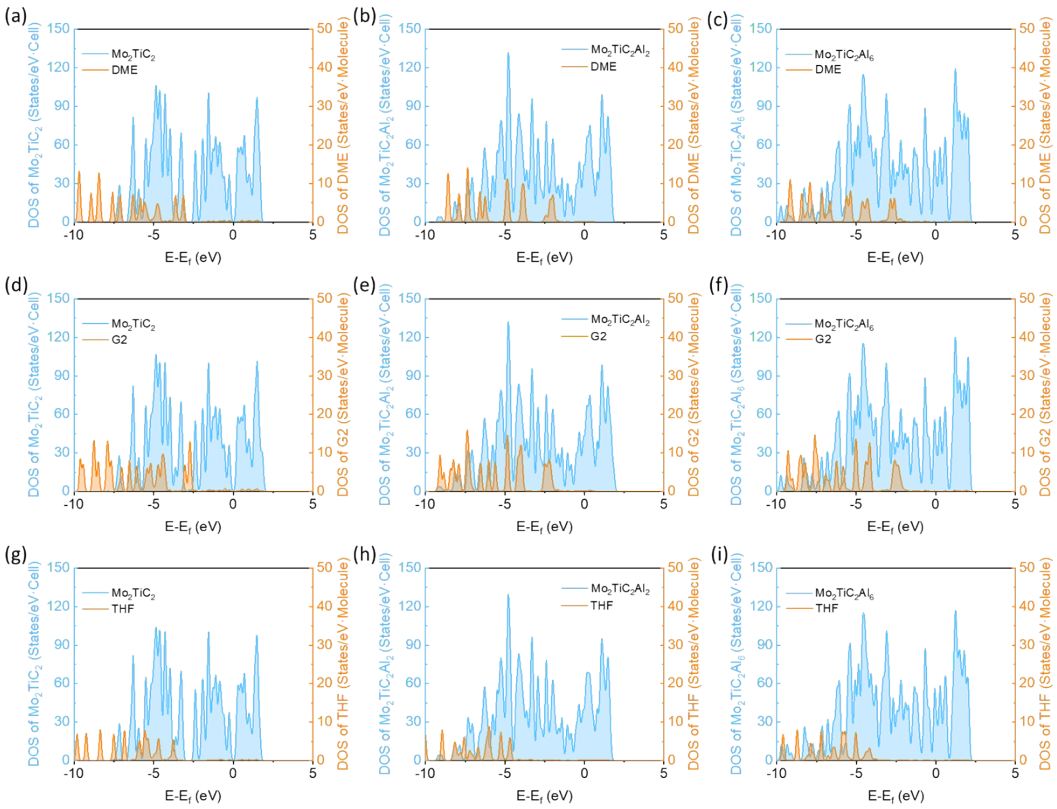

Figure S5. Electronic density of states of adsorbed molecule on Mo_2TiC_2, $Mo_2TiC_2Al_2$ and $Mo_2TiC_2Al_6$. (a)-(c) DME, (d)-(f) G2, (g)-(i) THF.

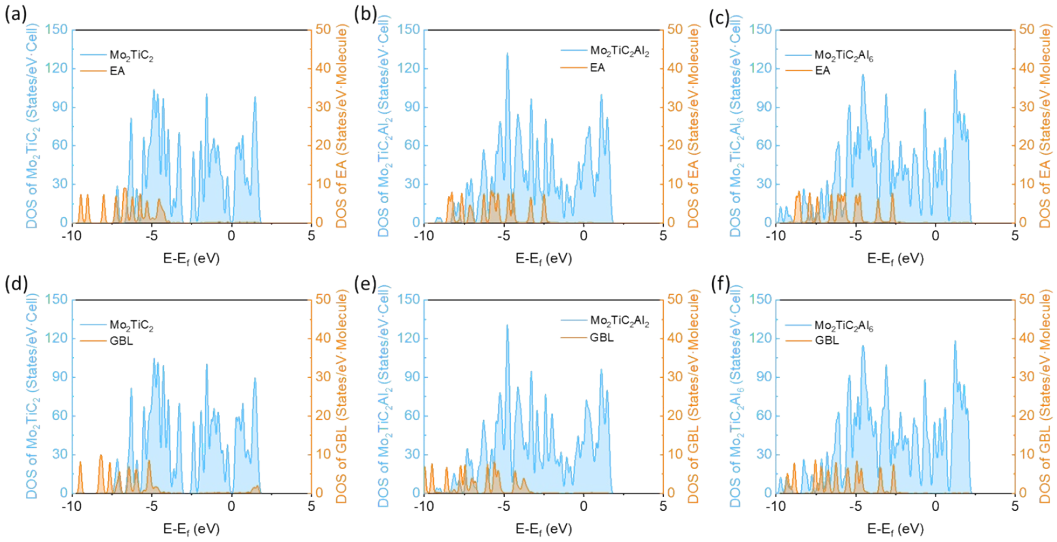

Figure S6. Electronic density of states of adsorbed molecule on Mo_2TiC_2, $Mo_2TiC_2Al_2$ and $Mo_2TiC_2Al_6$. (a)-(c) EA, (d)-(f) GBL.

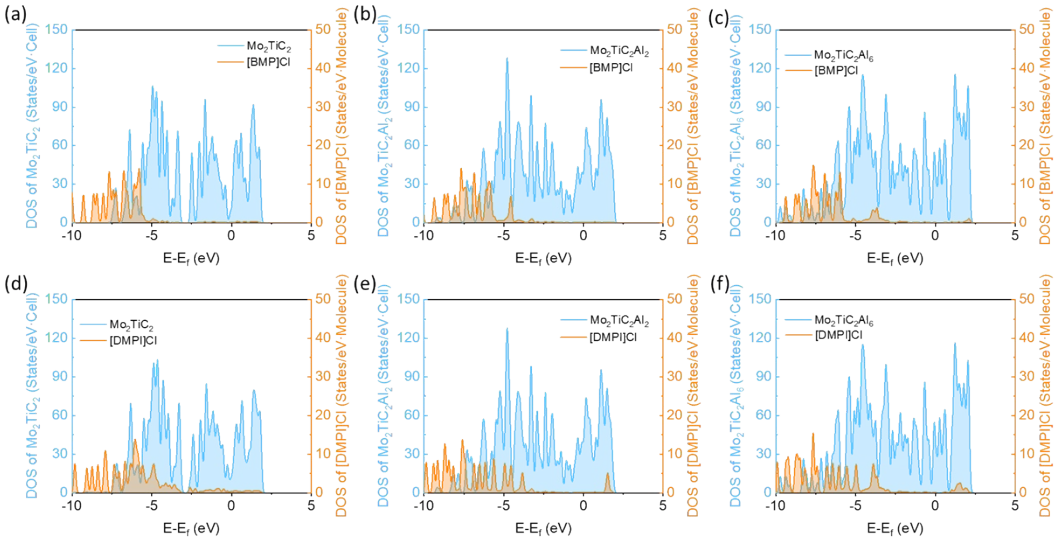

Figure S7. Electronic density of states of adsorbed molecule on Mo_2TiC_2, $Mo_2TiC_2Al_2$ and $Mo_2TiC_2Al_6$. (a)-(c) [BMP]Cl, (d)-(f) [DMPI]Cl.

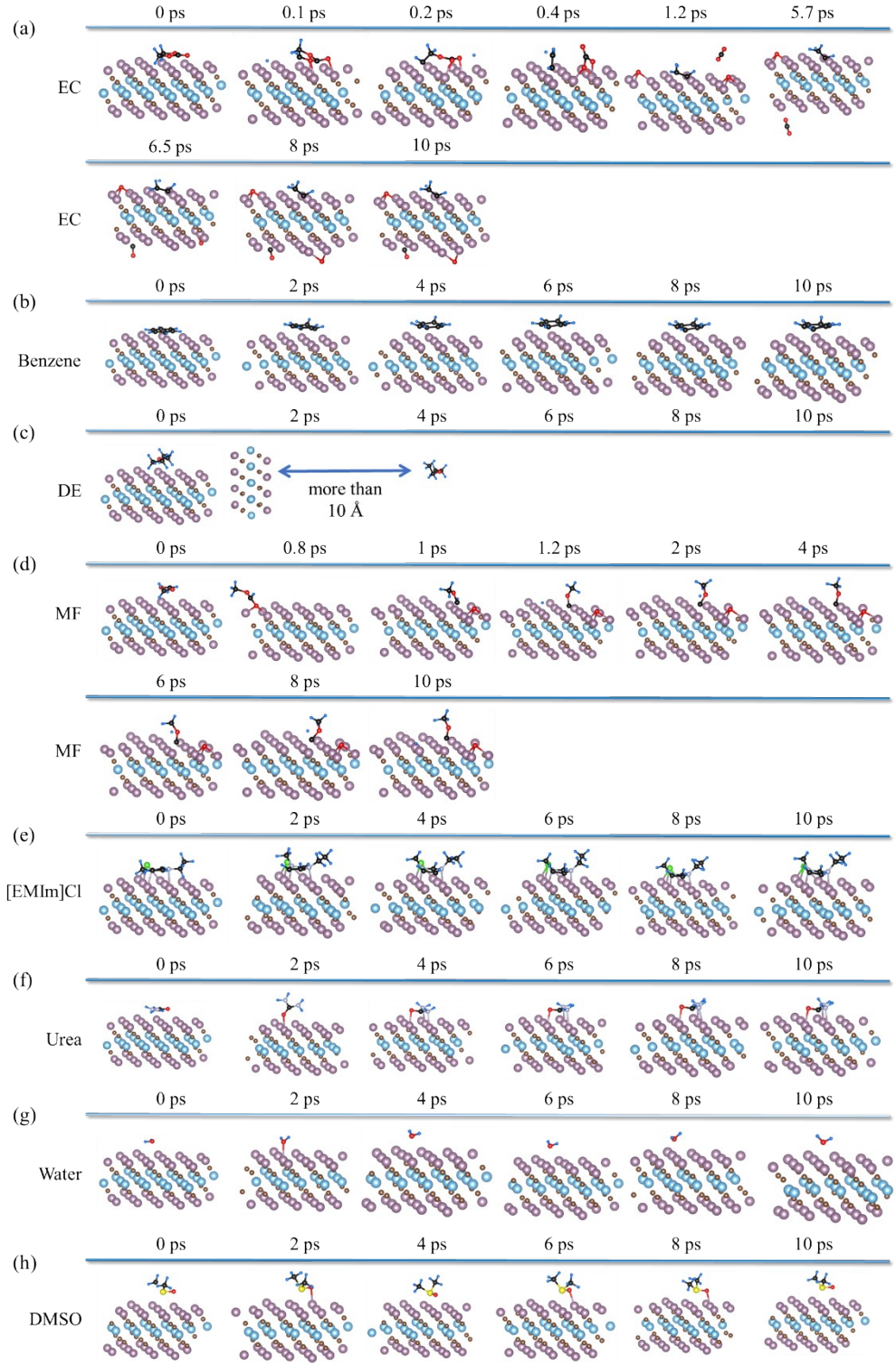

Figure S8. Snapshots of the adsorption of various representative solvents and ionic liquids on bare Mo_2TiC_2 monolayer at 300 K and different FPMD simulation times, including: (a) ethylene carbonate (EC), (b) aromatic hydrocarbons (benzene), (c) ethers (diethyl ether or DE), (d) carboxylic esters (methyl formate or MF), (e) ionic liquids ($[EMIm]^+Cl^-$), (f) urea, (g) water and (h) DMSO.

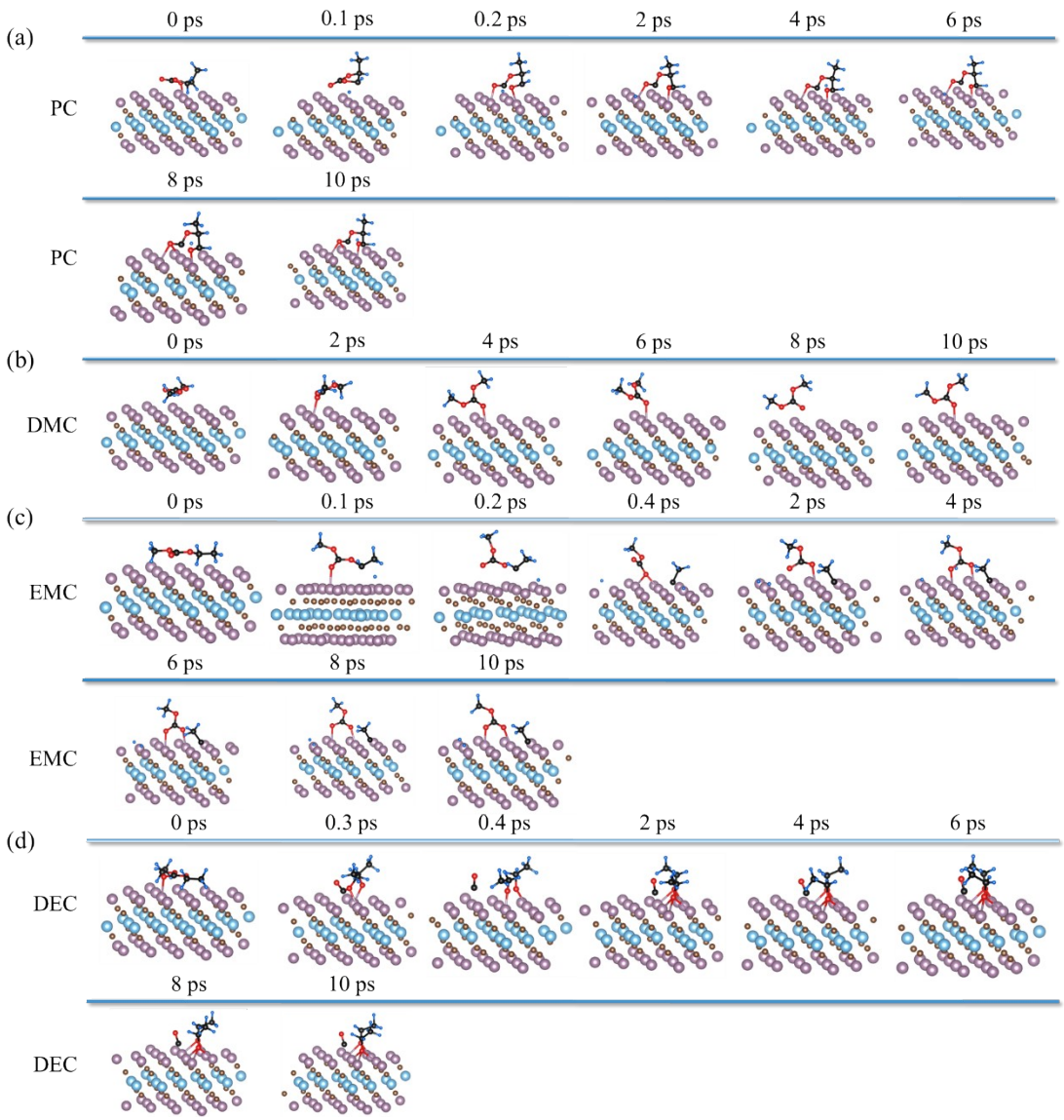

Figure S9. The AIMD simulation results for carbonates with Mo_2TiC_2: (a) PC, (b) DMC, (c) EMC, (d) DEC.

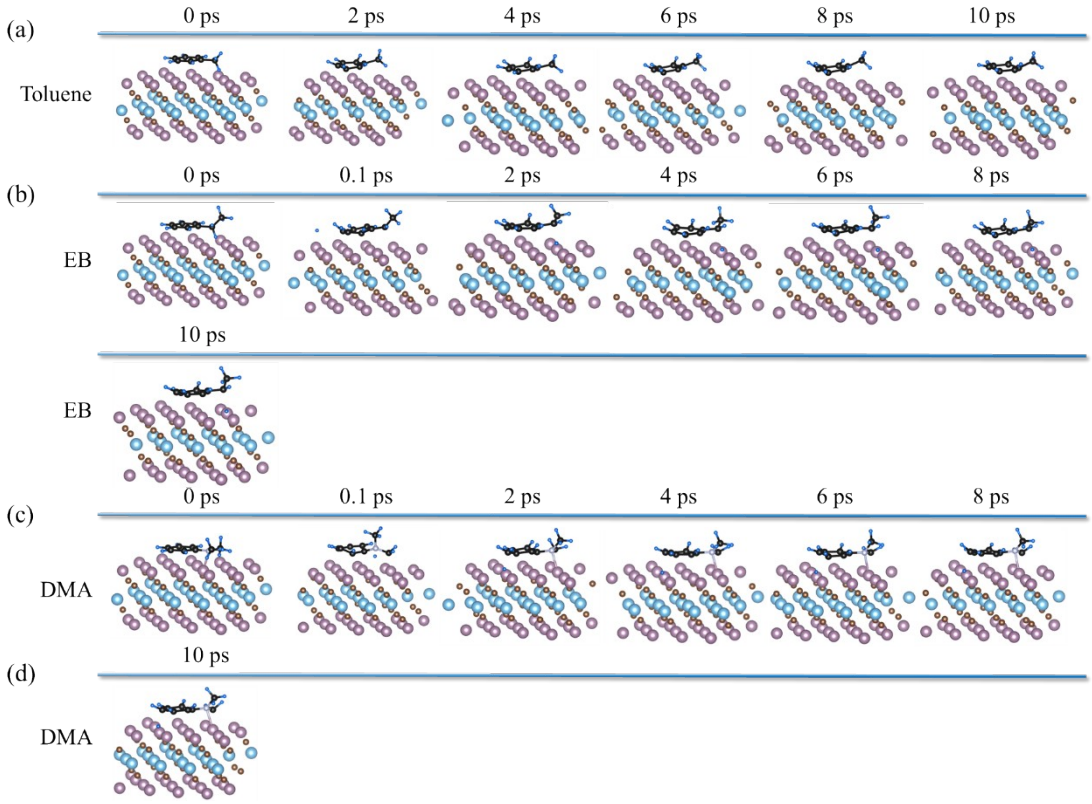

Figure S10. The AIMD simulation results for benzenes with Mo_2TiC_2: (a) Toluene, (b) EB, (c) DMA.

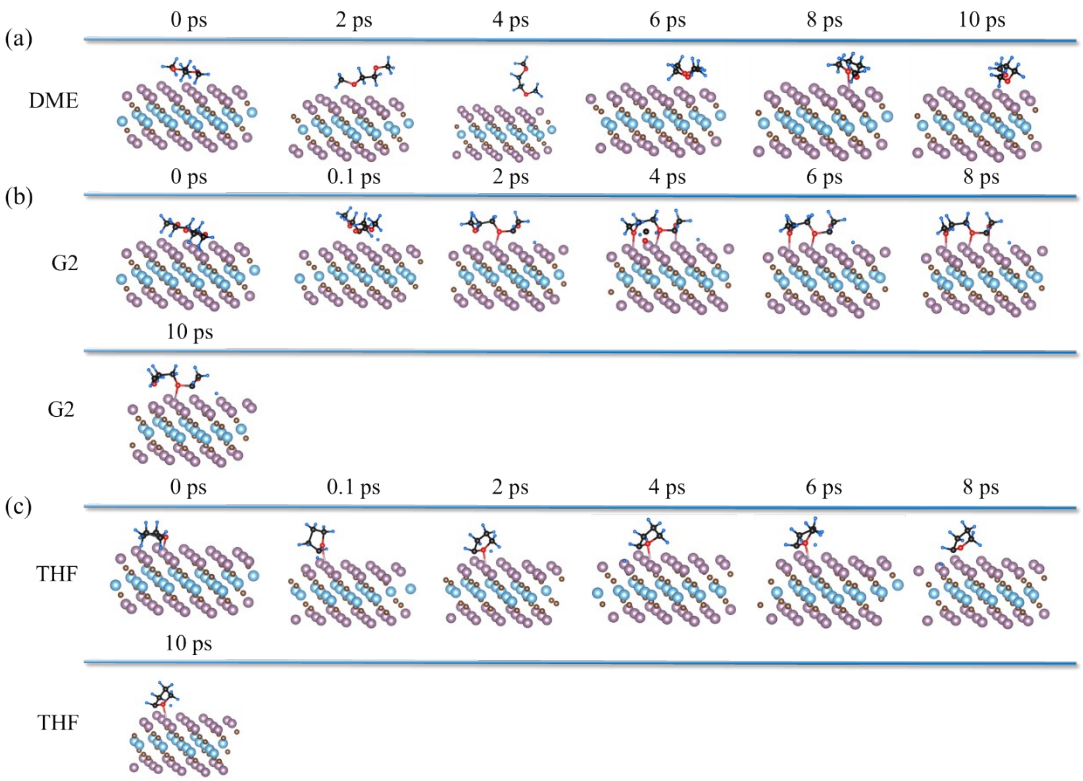

Figure S11. The AIMD simulation results for ethers with Mo_2TiC_2: (a) DME, (b) G2, (c) THF.

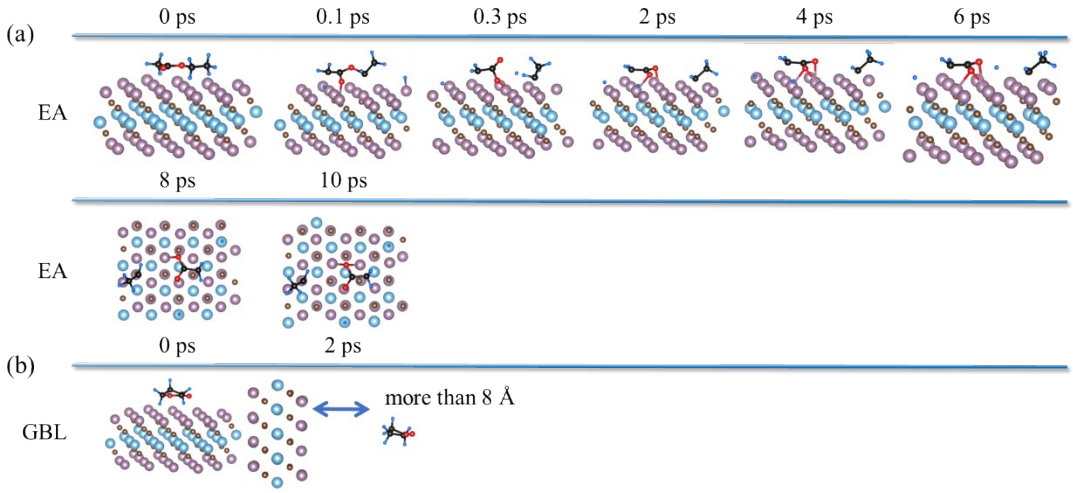

Figure S12. The AIMD simulation results for esters with Mo_2TiC_2: (a) EA, (b) GBL.

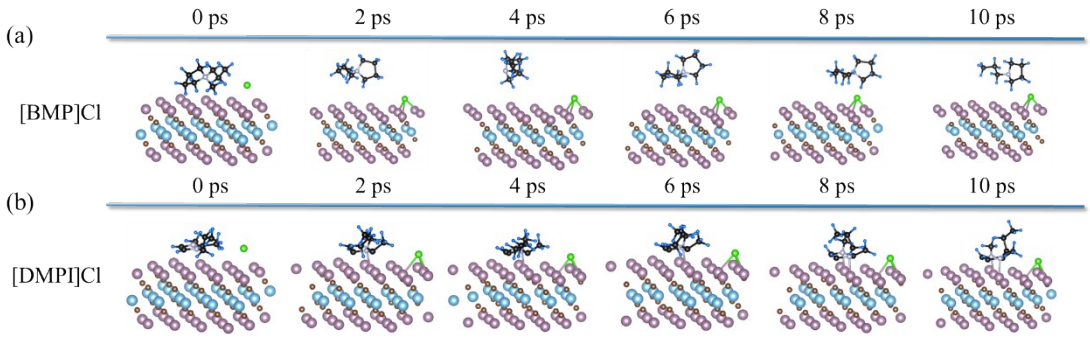

Figure S13. The AIMD simulation results for some ion liquids with Mo_2TiC_2: (a) [BMP]Cl, (b) [DMPI]Cl.

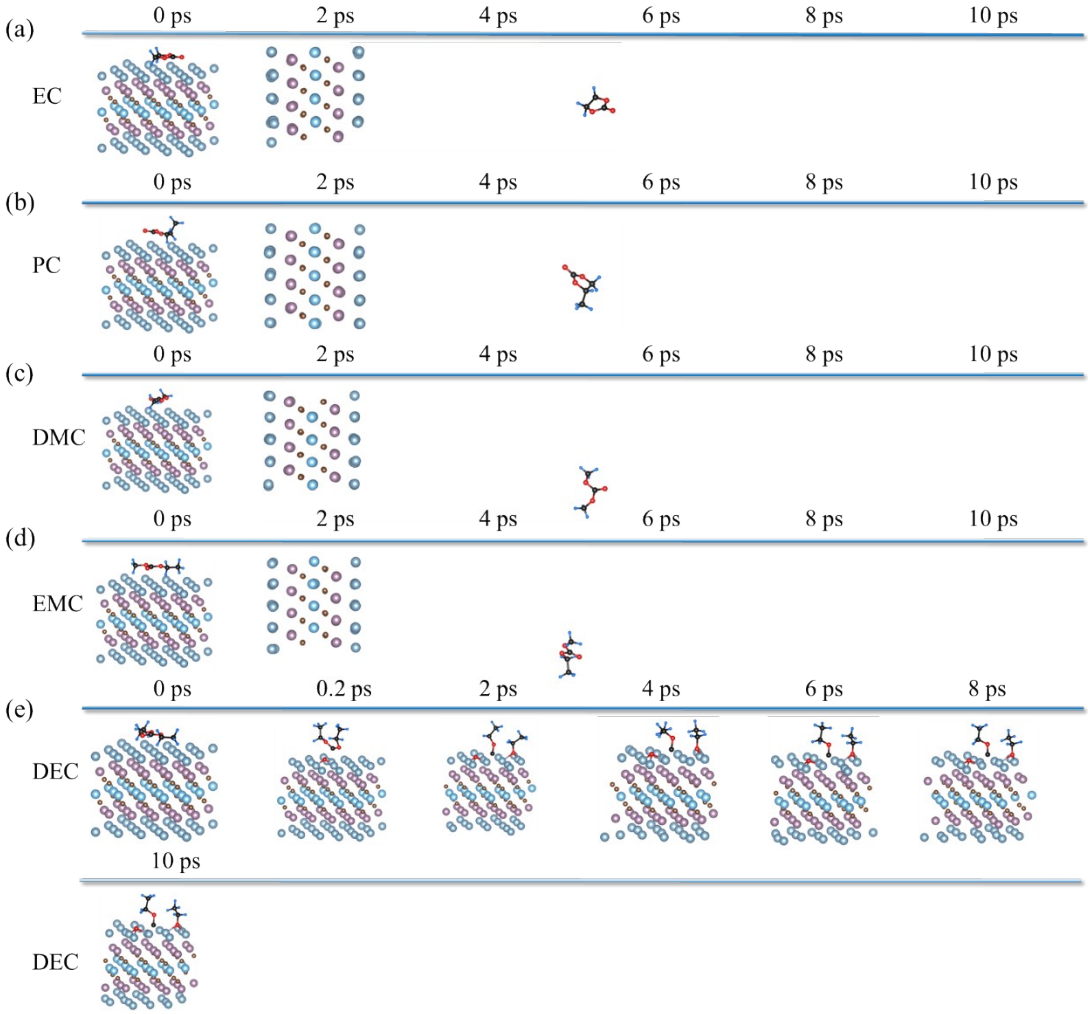

Figure S14. The AIMD simulation results for carbonate esters with $Mo_2TiC_2Al_2$: (a) EC, (b) PC, (c) DMC, (d) EMC, (e) DEC.

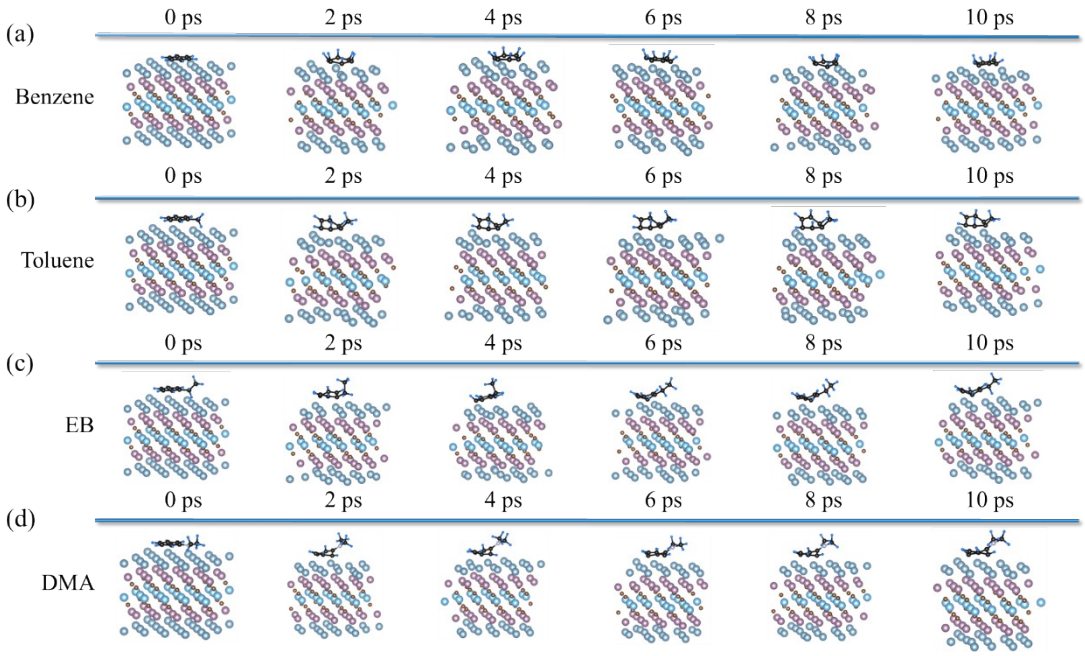

Figure S15. The AIMD simulation results for benzenes with $Mo_2TiC_2Al_2$: (a) benzene, (b) toluene, (c) EB, (d) DMA.

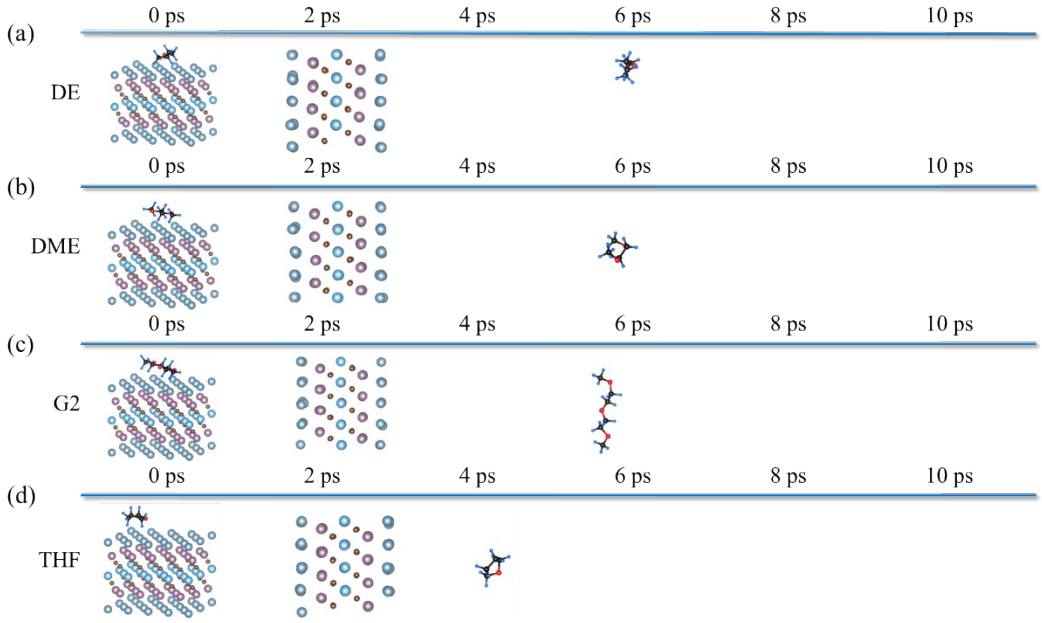

Figure S16. The AIMD simulation results for ethers with $Mo_2TiC_2Al_2$: (a) DE, (b) DME, (c) G2, (d) THF.

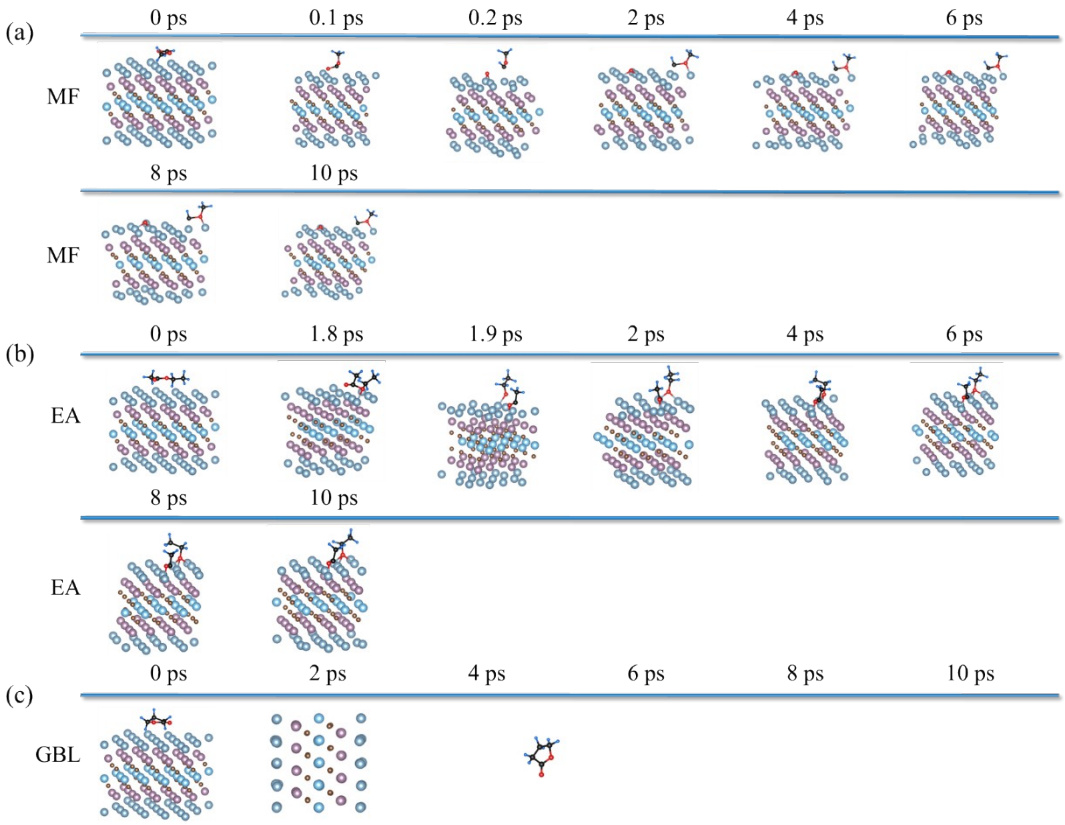

Figure S17. The AIMD simulation results for esters with $Mo_2TiC_2Al_2$: (a) MF, (b) EA, (c) GBL.

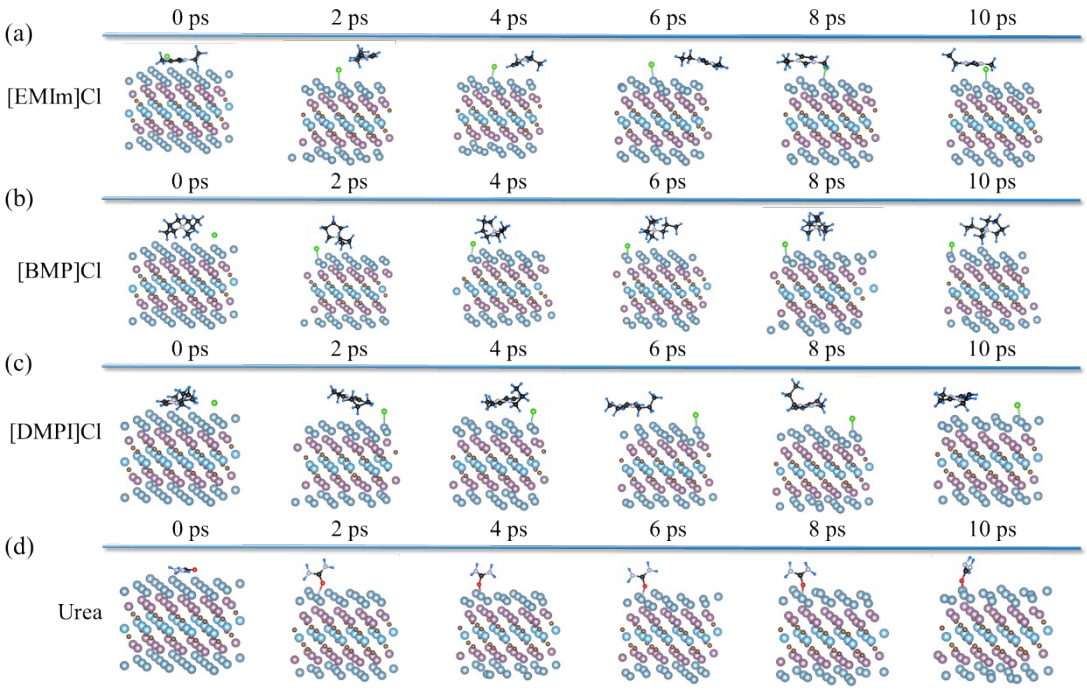

Figure S18. The AIMD simulation results for some ion liquids with $Mo_2TiC_2Al_2$: (a) [EMIm]Cl, (b) [BMP]Cl, (c) [DMPI]Cl, (d) urea.

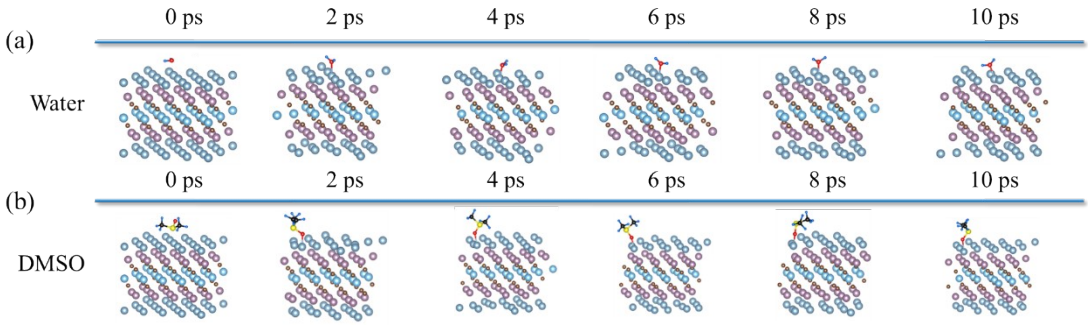

Figure S19. The AIMD simulation results for (a) water and (b) DMSO with $Mo_2TiC_2Al_2$.

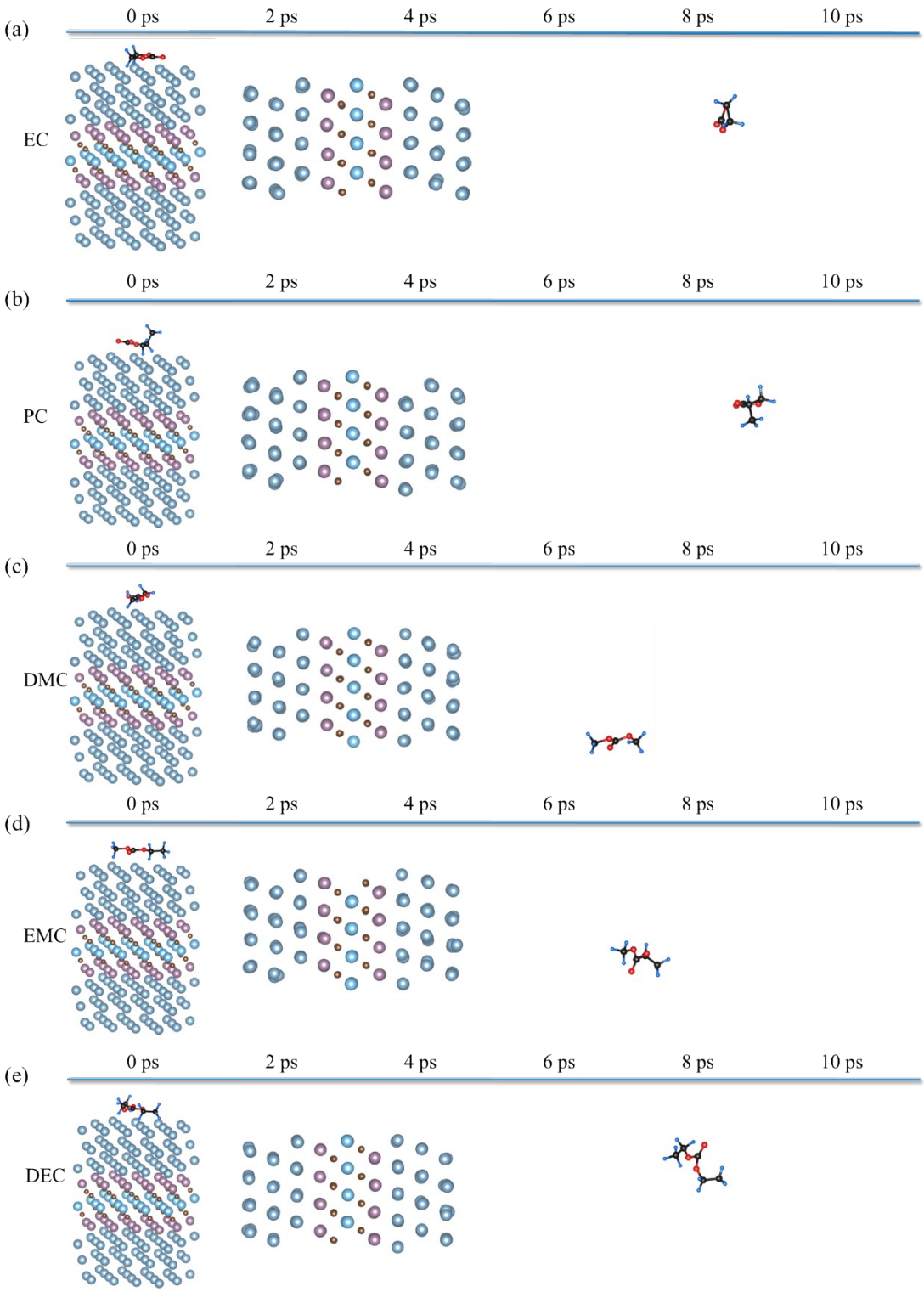

Figure S20. The AIMD simulation results for carbonate esters with $Mo_2TiC_2Al_6$: (a) EC, (b) PC, (c) DMC, (d) EMC, (e) DEC.

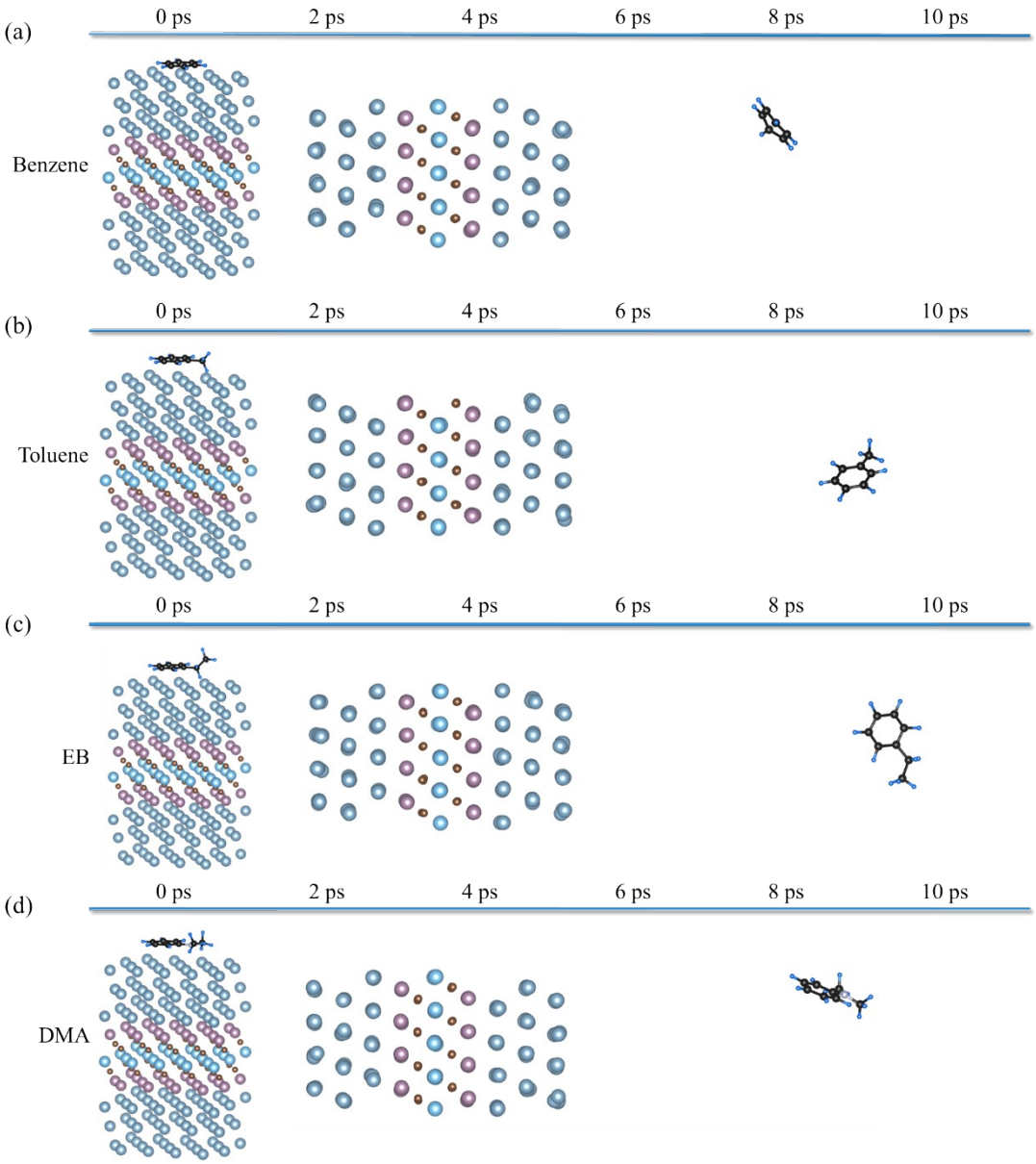

Figure S21. The AIMD simulation results for benzenes with $Mo_2TiC_2Al_6$: (a) benzene, (b) toluene, (c) EB, (d) DMA.

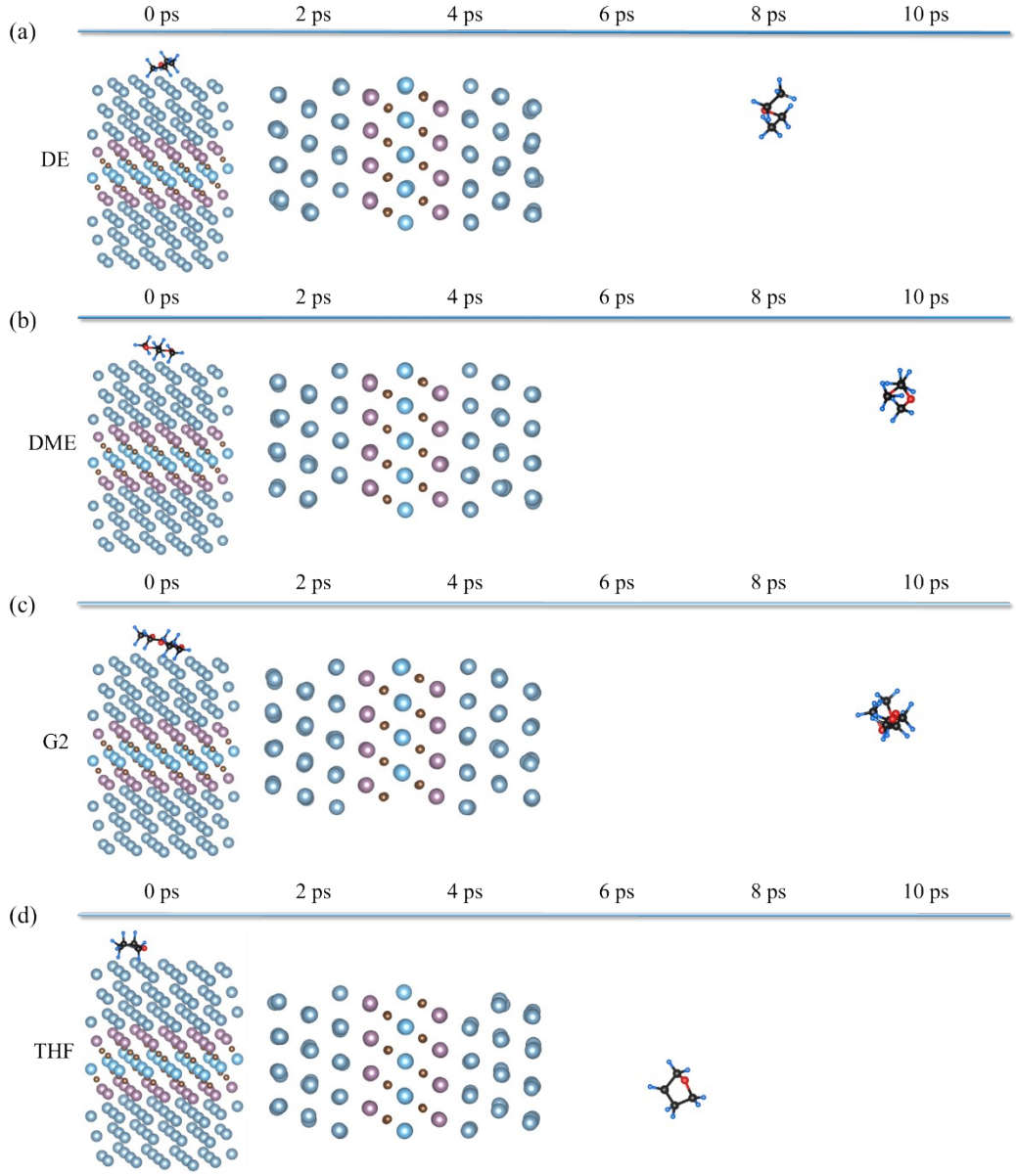

Figure S22. The AIMD simulation results for ethers with $Mo_2TiC_2Al_6$: (a) DE, (b) DME, (c) G2, (d) THF.

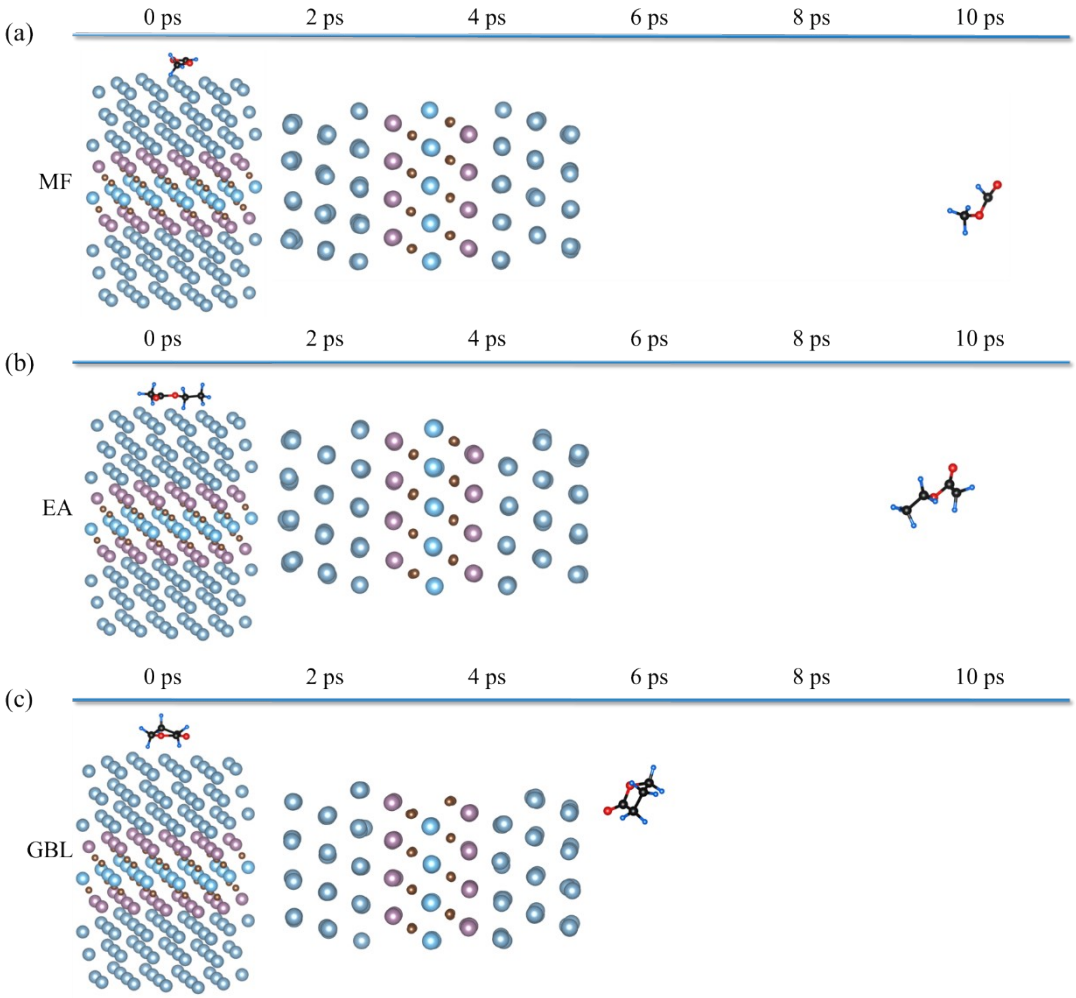

Figure S23. The AIMD simulation results for esters with $Mo_2TiC_2Al_6$: (a) MF, (b) EA, (c) GBL.

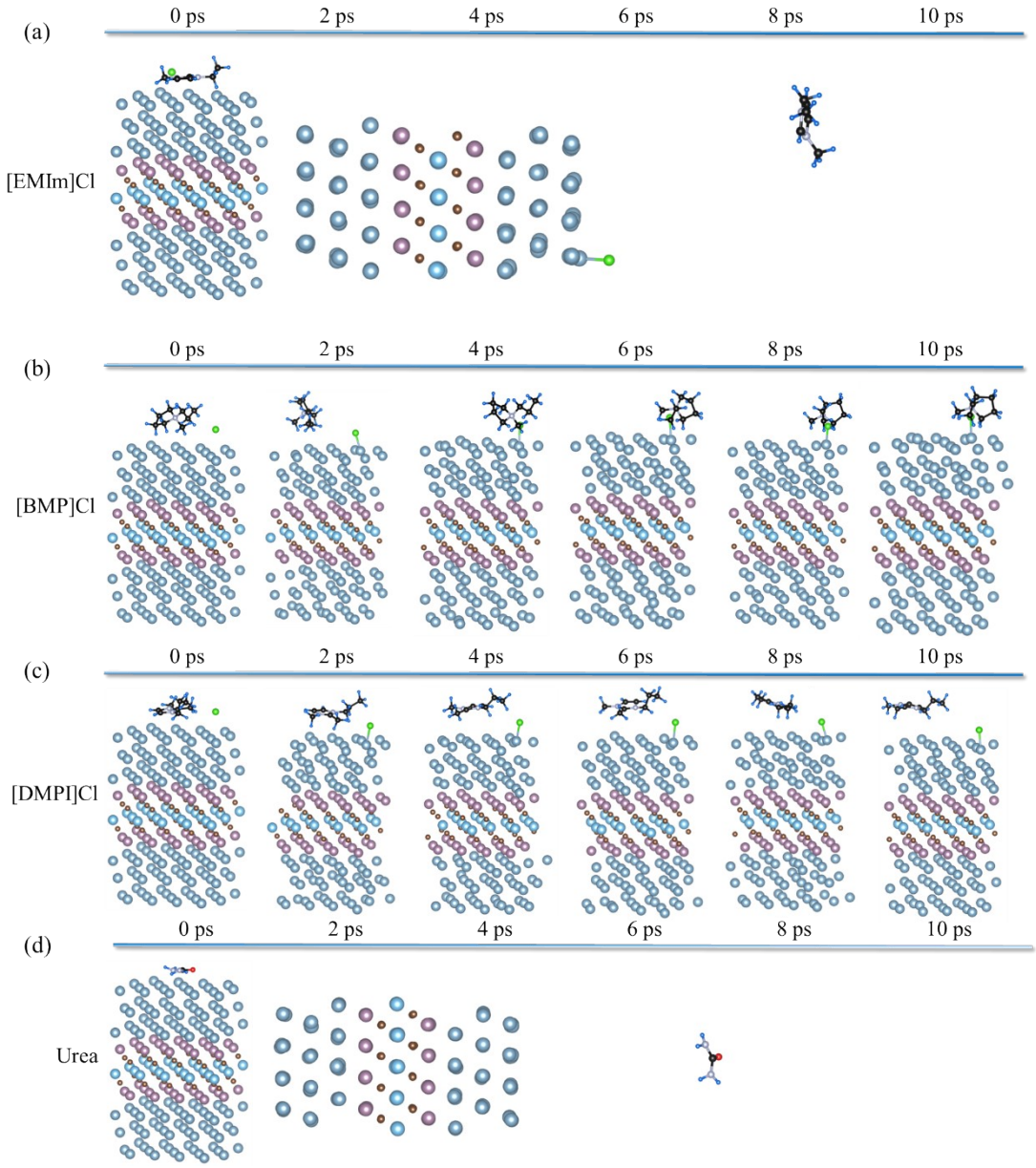

Figure S24. The AIMD simulation results for ion liquids with $Mo_2TiC_2Al_6$: (a) [EMIm]Cl, (b) [BMP]Cl, (c) [DMPI]Cl, (d) urea.

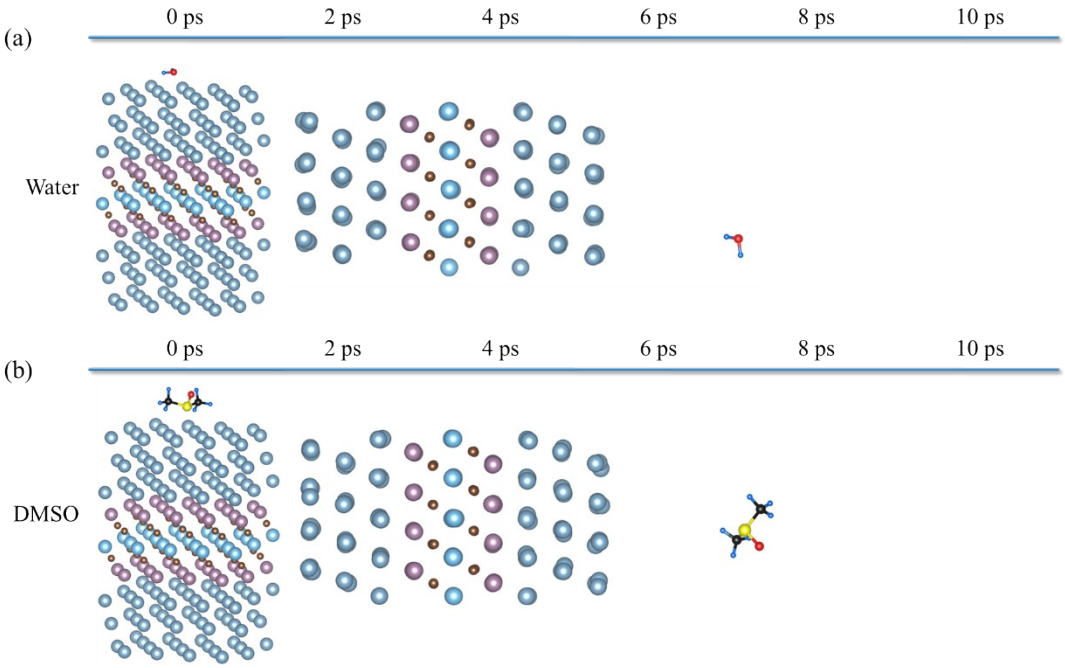

Figure S25. The AIMD simulation results for (a) water and (b) DMSO with $Mo_2TiC_2Al_6$.

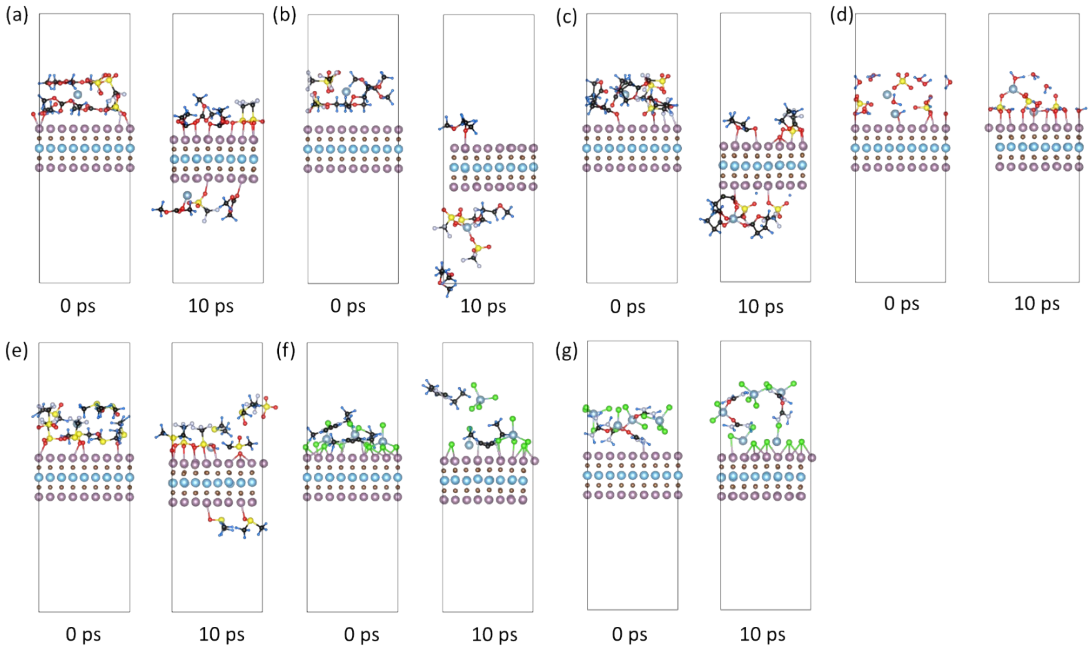

Figure S26. The AIMD simulation results of electrolytes on Mo_2TiC_2. (a) DMC-$Al(OTF)_3$, (b) DME-$Al(OTF)_3$, (c) GBL-$Al(OTF)_3$, (d) water-$Al_2(SO_4)_3$, (e) DMSO-$Al(OTF)_3$, (f) [EMIm]Cl-$AlCl_3$, (g) urea-$AlCl_3$.

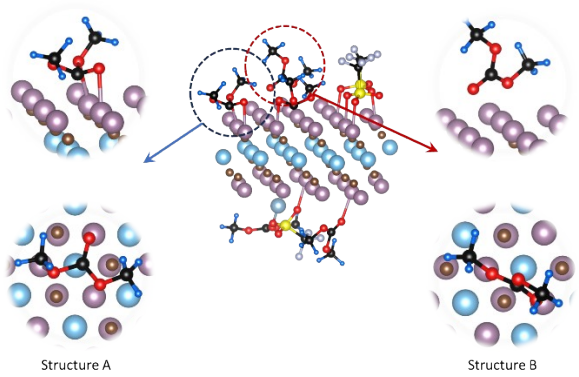

Figure S27. A snapshot representing the interface between the bare Mo_2TiC_2 monolayer and the DMC-$Al(OTF)_3$ electrolyte at 300 K from FPMD simulation.

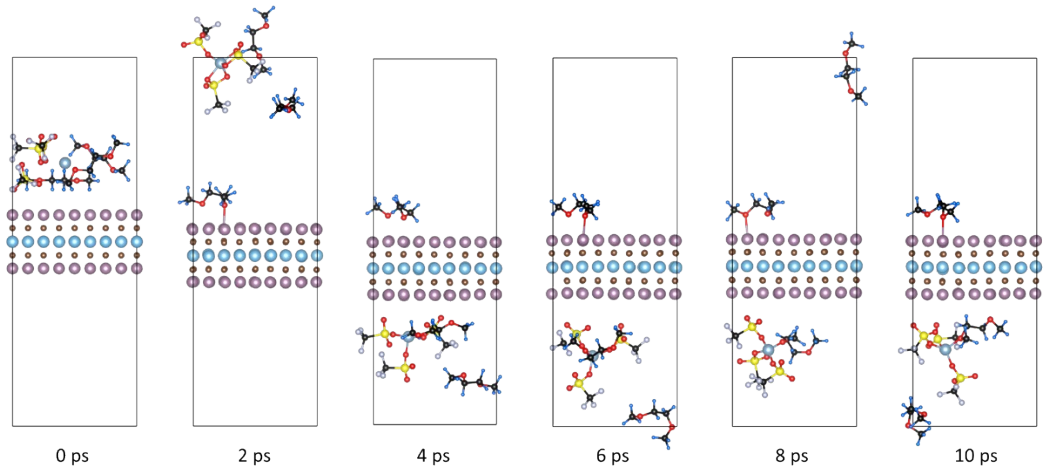

Figure S28. Selected snapshots showing the adsorption of DME-Al(OTF)$_3$ electrolyte on the bare Mo_2TiC_2 monolayer at different simulation times in FPMD simulation.