

Figure S1. Density of electronic states structure resolved by d-orbitals for Mo atoms and by p-orbitals for S atoms for A'-MoS₂.

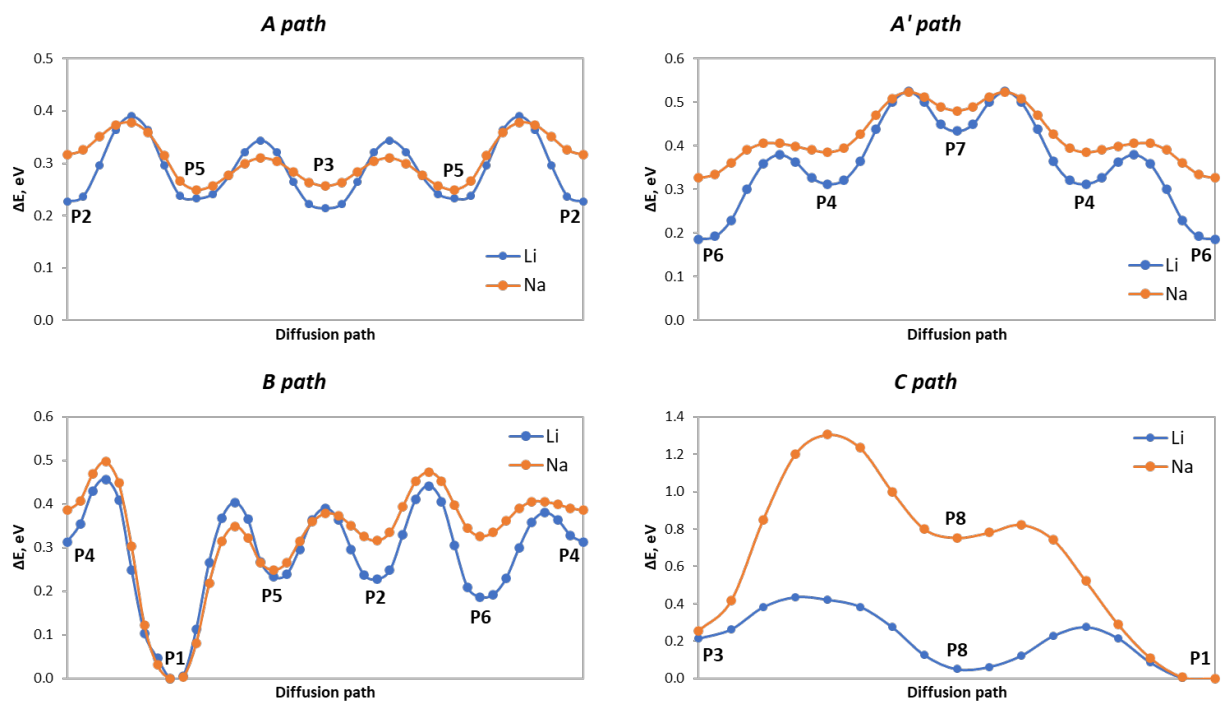


Figure S2. Diffusion energy profiles for Li (blue) and Na (orange) atoms diffusion barriers in different considered directions for A'-MoS₂.