About Stability of Hong-type NASICON Solid Electrolyte

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NASICON (Na Super Ionic CONductor) structure has high potentialities in diverse applications, such as refractory materials, sensors and solid electrolytes. Unfortunately, the stability and Na+ ion migration of NASICON have not been fully explored to grasp the fundamental characteristics. Therefore, we investigated the structural stability and ion conductivity of NASICON using density functional theory calculation. Four types of NASCION structure were considered according to the ratio of Si and P atoms (*i.e.*, Si_3, Si_2P (i.e., Hong-type), SiP_2, P_3). We found that formation of tetrahedral Si/P vacancy was relatively favorable through vacancy formation energy calculation. Especially, the P vacancy induced the dumbbell-shaped oxygens in the Na^+ ion channel, which could obstruct the Na^+ ion migration. Hydronium exchange reaction, which degrades NASICON by blocking the Na^+ ion channel and causing the structural deformation, was calculated in water and seawater environments. We found that the reactivity of NASICON decreased in seawater condition.