Chemical bonding of lithium and calcium ions intercalated into MS_2 (M = Ti, V)

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Transition metal dichalcogenides (TMDs) have been extensively studied as an active material for secondary batteries [1]. However, there are few studies on chemical bonding between TMDs and atoms intercalated into them. In this study, bond overlap population (BOP) and net charge of atoms in four types of cluster structures, $X_{13}M_{26}S_{48}$ (X = Li, Ca and M = Ti, V), were investigated by DV-Xα molecular orbital method. In $X_{13}Ti_{26}S_{48}$, the BOP indicating the covalency between Li and S was greater than that between Ca and S. In contrast, in $X_{13}V_{26}S_{48}$, the former was smaller than that the latter. On the other hand, the BOP between Ti and S was smaller in $Li_{13}Ti_{26}S_{48}$ than in $Ca_{13}Ti_{26}S_{48}$, and the BOP between V and S is greater in $Li_{13}V_{26}S_{48}$ than in $Ca_{13}V_{26}S_{48}$. Additionally, the ionicity between X and M was smaller in $Li_{13}M_{26}S_{48}$ than in $Ca_{13}M_{26}S_{48}$. This work provides useful information for understanding the electrode reaction of secondary batteries using TDMs as an active material.

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Reference

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