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Ab initio **study of layered chromium disulfide (CrS_2) toward a new anode material for Li-ion batteries** SEOUNG-HUN KANG, YOUNG-KYUN KWON, Kyung Hee University — There has been considerable interest in use of transition-metal disulfides, such as MS_2 (M=Mo, W), as new anode materials in Li-batteries to improve their battery performance. Since CrS_2, if synthesized, would be much lighter than MoS_2 or WS_2, it would exhibit higher Li capacity. To verify this expectation, we investigate the adsorption and diffusion properties of Li on layered Cr_2 and its Li capacity using DFT implemented with van der Waals correction. We thoroughly search for variuos Li adsorption sites, on which the binding energies are higher than Li clustering energy ($\sim$ 1.6 eV). Based on the these calculations, we identify the diffusion paths and barriers of Li atoms within the layered CrS_2 as well as on a free-standing single-layer of CrS_2. We find that Li atoms exhibit almost free intra-layer diffusion resulting in an improved mobility of Li at room temperature, while inter-layer diffusion is difficult to occur. We also estimate the Li-capacity of the CrS_2 by evaluating the energy gain as well as the average binding energy while intercalating more Li atoms. We find that CrS_2 can have larger Li-capacity than graphite, which is being widely used for anode material, implying that CrS_2 may be a good candidate for Li-battery electrode.

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