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A First-Principles Study of the Potassium Insertion in Crystalline Vanadium Oxide Phases as Possible Potassium-Ion Battery Cathode Materials.

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Potassium (K) is an element almost as abundant as sodium and with a low standard redox potential comparable to that of Li/Li^+, which makes potassium ion batteries attractive and attracting increasing research interest. Especially in the investigation of suitable cathode materials some progress was made. A group of possible cathode materials which has not yet been studied in detail are crystalline vanadium oxides, although their excellent intercalation properties are known for a variety of other alkali and alkaline earth elements, including Li, Na, Mg, and Al. Since numerous vanadium oxides with different stoichiometries and with distinct phases exist in close proximity in phase space, a systematic experimental study of all possible intercalation compounds and a rationalization of the performance (insertion potentials, capacities) of different phases and of the mechanism of insertion is difficult. That is why it is important to use ab initio methods to investigate and pre-screen suitable electrode materials and make accurate predictions with regard to the above properties in a systematic way. In this study, four promising vanadium oxide phases (α-V_2O_5, β-V_2O_5, bronze- and rutile-type VO_2), which are shown in Figure 1, are investigated from first principles as potential electrode materials for K ion batteries. Insertion energetics and diffusion barriers are computed. Our results show that the monoclinic β-V_2O_5 provides the lowest (strongest) insertion energies for K and the lowest diffusion barriers compared to orthorhombic α-V_2O_5, bronze and rutile VO_2. While three of these phases show an energetically favorable potassiation and relatively small diffusion barriers, VO_2(R) is predicted to be incapable of electrochemical K incorporation.

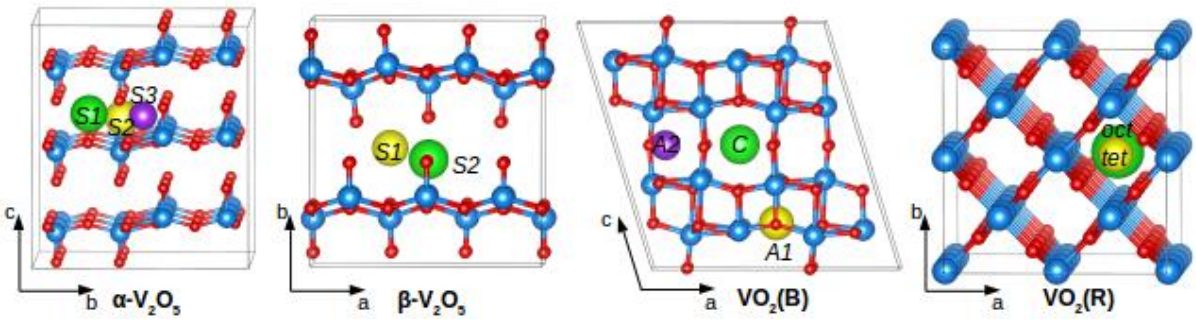

Figure 1. α-V_2O_5, β-V_2O_5, VO_2(B) and VO_2(R) (from left to right) simulation cells with possible insertion sites. The red spheres denote O, the blue spheres V positions, possible K insertion sites are denoted by green, yellow and purple spheres and their designations are given. Crystallographic directions along front face of cell are indicated.