Electrochemical and theoretical investigations of  $Na_2Ti_3O_7$  and  $Na_2Ti_6O_{13}$  as  $Na^+$  intercalation anodes

Anthony G. Dylla, Penghao Xiao, Graeme Henkelman and Keith J. Stevenson

Department of Chemistry and Biochemistry, The University of Texas at Austin 1 University Station Austin, TX 78712

Potential problems with lithium availability in the future may demand the use of other charge storage chemistries for high capacity applications such as grid storage. Rechargeable Na<sup>+</sup> batteries could help meet this demand due to its ubiquity throughout nature. While several high voltage cathodes have been identified for Na<sup>+</sup> rechargeable batteries, viable low voltage anodes have been scarily identified. Here we present electrochemical and theoretical investigations of two sodium titanates,  $Na_2Ti_3O_7$  and  $Na_2Ti_6O_{13}$  as low voltage (ca. 0.5 V vs Na<sup>+</sup>/Na<sup>0</sup>) Na<sup>+</sup> intercalation hosts. At 800 °C the layered  $Na_{2}Ti_{3}O_{7}$  condenses to  $Na_{2}Ti_{6}O_{13},$  which exhibits a more 3-D microporous structure. These structural changes may have implications for understanding Na<sup>+</sup> insertion mechanisms and will be explored through combined experimental and density functional theory (DFT) studies.

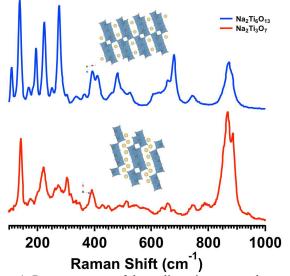


Figure 1. Raman spectra of the sodium titanates under investigation along with their crystal structures.