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Rational design of TiO_2-based anode materials using computer modeling

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Abstract – On the basis of advanced computer simulations a relationship between the structure and intercalation behaviour of titanates is established, which is based on the charge transfer occurring upon intercalation. Understanding of the relationship is used for screening of prospective morphologies and prediction of the effect of the nanoscale on the intercalation properties.

Battery research has always been dominated by the search for novel electrode materials to enhance uptake and transport of Li-ions and, hence, high energy and power density. To achieve efficient design and optimization of advanced electrode materials, typically nanostructured transition metal oxides, understanding of the relation between the intercalation and structural properties of the host is vital. Despite widespread interest and massive amount of experimental and theoretical research, up to date the structure-property relationship has not been established. Using titanium dioxide based materials as an example and advanced computer simulation techniques as a tool , we demonstrate that this relationship is based on the charge transfer occurring upon intercalation. We summorize this realtionship in a simple model relating the structure of undoped titanates to the expected intercalation properties of the bulk. Using this model, we identify TiO_2-B as a material to deliver the highest energy density among titanates.Furthermore, by considering the local connectivity and hence stability, we estimate the relative intercalation potential of titanates to identify material that intercalates Li-ions at significantly lower potential than current state of the art anodes in the same concentration range ($Li_{0.5}TiO_2$ (R)).

Recently, it has been demonstrated that Li-intercalation behaviour of some transition metal oxides including rutile and brookite structured TiO_2 depends critically on the size of their particles [1,2]. These materials show almost no Li-uptake in polycrystalline form, but intercalate Li-ions to high concentrations into the nanosize particles. Also, specially tailored nanoparticles may exhibit a completely different sequence of phase transformations. We show that the model developed here can be used to predict effect of the nanoscale on the intercalation behaviour of various titanates, including their insertion capacity, phase boundaries and transport properties, providing a rationale for the observed behaviour.

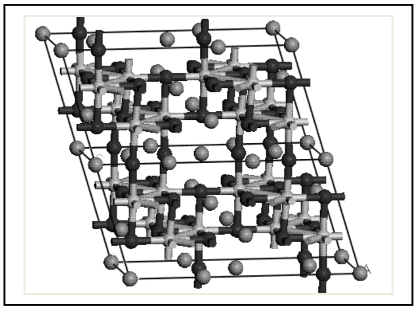

Figure 1: Predicted structure of $Li_{1.25}TiO_2$(B)

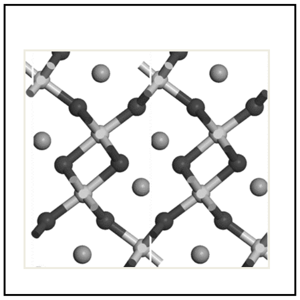

Figure 2: Predicted structure of $LiTiO_2$(R)

References

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[2] M. A. Reddy, M.S. Kishore, V. Pralong, U.V. Varadaraju, B. Raveau, Electrochem Solid-State Lett., 10, (2007) A29 (2007)