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Theoretical Investigation of oxides for batteries and fuel cell applications PANCHAPAKESAN GANESH, ANDREW A. LUBIMTSEV, JANAKIRAMAN BALACHANDRAN, Center for Nanophase Materials Sciences, ORNL — I will present theoretical studies of Li-ion and proton-conducting oxides using a combination of theory and computations that involve Density Functional Theory based atomistic modeling, cluster-expansion based studies, global optimization, high-throughput computations and machine learning based investigation of ionic transport in oxide materials. In Li-ion intercalated oxides, we explain the experimentally observed (Nature Materials 12, 518522 (2013)) 'intercalation pseudocapacitance' phenomenon, and explain why Nb_2O_5 is special to show this behavior when Li-ions are intercalated (J. Mater. Chem. A, 2013,1, 14951-14956), but not when Na-ions are used. In addition, we explore Li-ion intercalation theoretically in $VO_2(B)$ phase, which is somewhat structurally similar to Nb_2O_5 and predict an interesting role of site-trapping on the voltage and capacity of the material, validated by ongoing experiments. Computations of proton conducting oxides explain why Y-doped $BaZrO_3$, one of the fastest proton conducting oxide, shows a decrease in conductivity above 20% Y-doping. Further, using high throughput computations and machine learning tools we discover general principles to improve proton conductivity. Acknowledgements: LDRD at ORNL and CNMS at ORNL

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