Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

**Combinatorial Libraries of Transition Metal Oxides Using an Ab Initio High Throughput Approach**[1] GUO LI, QIMIN YAN, Lawrence Berkeley Natl Lab, PAUL NEWHOUSE, LAN ZHOU, JOHN GREGOIRE, California Institute of Technology, JEFFREY NEATON, Lawrence Berkeley Natl Lab; UC-Berkeley; Kavli Energy NanoSciences Institute at Berkeley — Using the results of first-principles calculations and data from the Materials Project (materialsproject.org), we have developed a simple but efficient scheme to theoretically simulate phase coexistence in experimental combinatorial libraries as a function of composition and temperature. In our approach, each experimental sample in a combinatorial library at a fixed composition is considered as a mixture of all the known compounds; and the compound concentrations are determined from calculations of their compositions and relevant thermodynamic potentials. Consequently, multiple compounds can be identified in every sample. To test our approach, we studied the pseudobinary library MnxV(1-x)Oy, and found that, together with those stable compounds predicted in a phase diagram, some of the above-convex-hull compounds, which are viewed unstable, also play a significant role in the combinatorial library. We validated our approach via comparison of calculated X-ray diffraction spectra for multiple phases and recent measurements.

[1]This work supported by DOE (the JCAP under Award number DE-SC000499 and the Molecular Foundry of LBNL), and computational resources provided by NERSC.

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Date submitted: 05 Jan 2015 Electronic form version 1.4