Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Oxygen transport in ceria: a first-principles study[1] SIMAK SERGEI, Linkoping University, Linkoping, Sweden — Ceria (CeO2) is an important material for environmentally benign applications, ranging from solid-oxide fuel cells (SOFC) to oxygen storage [1-2]. The key characteristic needed to be improved is the mobility of oxygen ions. Optimization of ionic transport in ceria has been the topic of many studies. In particular, it has been discovered how the ionic conductivity in ceria might be improved by choosing the proper kind and concentration of dopants [3]. In this presentation we will approach the problem from a different direction by adjusting structural parameters of ceria via the change of external conditions. A systematic first-principles study of the energy landscape and kinetics of reduced ceria as a function of external parameters reveals a physically transparent way to improve oxygen transport in ceria.

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[1]We would like to thank the Swedish Research Council, (VR) for financial support and the Swedish National Infrastructure for Computing (SNIC) for computational resources. Thanks to the Swedish Government Strategic Research Area Grant in Materials Science

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Date submitted: 21 Nov 2011 Electronic form version 1.4