Oxygen Activation and Dissociation on Transition Metal Free Perovskite Surfaces

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Short Biography

Aleksandar Staykov obtained M. Sc. degree in Organic Chemistry from Sofia University, Bulgaria in 2002. In 2006, he obtained his Ph. D. degree in Physical Chemistry from Wilhelm Ostwald Institute, Leipzig University, Germany with supervisors Prof. Dr. h. c. Nikolai Tyutyulkov and Prof. Fritz Dietz. During his Ph. D. he was awarded with DAAD fellowship for study and research in Germany. From 2006-2011 Dr. Staykov is a postdoctoral researcher in the Institute for Materials Chemistry and Engineering, Kyushu University, Japan with supervisor Prof. Kazunari Yoshizawa. During this period, he was awarded with JSPS fellowship for research in Japan, CSJ presentation award, and BCSJ best article award. From 2011 Dr. Staykov is appointed as an assistant professor at the International Institute for Carbon Neutral Energy Research, Kyushu University. In 2014, he was promoted to associate professor and in 2015 he received a permanent faculty position and became a part of the department of Applied Chemistry, Kyushu University. Dr. Aleksandar Staykov is lecturing the course of Thermodynamics for the second-year Applied Chemistry students. Dr. Staykov works actively in the field of theoretical chemistry and computational materials science. He has 59 peer-reviewed publications in impacted scientific journals, such as, ASC Nano, J. Am. Chem. Soc., Chem. Mater., J. Phys. Chem. C, J. Mater. Chem. A., etc. He has collaborated and published together with renown experimentalists: Prof. Ben Feringa (2016 Nobel Prize in Chemistry), Prof. Klaus Mullen (Max Plank Institute for Polymer Science), Prof. John Kilner (Imperial College London), Dr. Brian Somerday (Sandia National Lab), Prof. Tatsumi Ishihara (Kyushu University).

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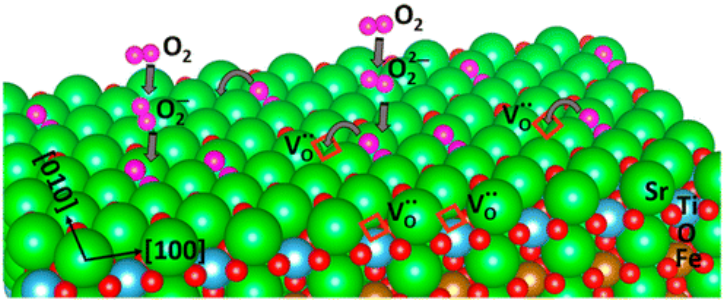
Abstract

Density functional theory and low energy ion scattering spectroscopy were applied to study the mechanism of oxygen dissociation on the SrO-terminated surfaces of strontium titanate ($SrTiO_3$) and iron-doped strontium titanate ($SrTi_{1-x}Fe_xO_{3-\delta}$). Our study reveals that while O_2 dissociation is not favored on the SrO-terminated perovskite surface, oxygen vacancies can act as active sites and catalyze the O–O bond cleavage. Electron transfer from lattice oxygen atoms to the O_2 molecule, mediated by the subsurface transition metal cations, plays an important role

in the resulting formation of surface superoxo species. The O_2 molecule dissociates to produce oxygen ions, which are incorporated into the perovskite lattice, and highly active oxygen radicals on the perovskite surface, which further recombine to O_2 molecules. Our focus on the SrO-terminated surface, rather than the TiO_2 layer, which is presumed to be more catalytically active, was driven by experimental observation using low energy ion scattering spectroscopy, which reveals that the surface of $SrTiO_3$ after high temperature heat treatment is SrO-terminated, and hence this is the surface that is technologically relevant for devices such as solid oxide fuel cells (SOFCs). Our study demonstrates that although the more active BO_2-perovskite layer is not exposed at the gas–solid interface, the SrO-terminated surfaces also actively participate in oxygen exchange reaction [1,2].



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