Lattice oxygen participation mechanism for the oxygen evolution reaction on perovskites

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In this seminar, I would like to talk about the importance of considering lattice oxygen participation during the oxygen evolution reaction (OER) on ABO_3 perovskites. Based on density functional theory calculations, I will discuss the electronic origin and kinetic feasibility of surface lattice oxygen participating in O_2 formation via non-electrochemical pathways. I will then show that the lattice oxygen participation mechanism (LOM) can lead to higher OER activity than the conventional adsorbate evolution mechanism (AEM) by minimizing the thermodynamically required overpotential. The OER activity volcano for AEM is universal for all perovskites whereas that for LOM depends on the identity of the A cation in ABO_3. This explains experimental observations that recently discovered perovskites such as $Pr_{0.5}Ba_{0.5}CoO_{3-x}$ and $SrCoO_{3-x}$ show higher OER activities than the conventionally predicted optimum compounds such as $LaNiO_3$ and $SrCoO_3$. Based on our activity volcano that considers both AEM and LOM, several new perovskite materials are predicted to be highly active for OER via LOM.