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Mechanical Engineering Lecture in Micro/Nano Engineering

Molecular Scale Understanding and Design of Active-Oxygen Materials for Solid Oxide Fuel Cells

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Active-oxygen materials have the ability to readily transport and exchange oxygen with the environment, and this capability gives them a critical role in many existing and developing technologies, including solid oxide fuel cells (SOFCs), gas separation membranes, oxygen sensors, chemical looping devices, and memristors. However, the molecular scale mechanisms by which these materials exchange oxygen with the gas phase are often poorly understood, inhibiting materials design and optimization. In this talk I will discuss my work on applications of active-oxygen materials for Solid Oxide Fuel Cells (SOFCs). These devices extract energy from fuels electrochemically, and offer a clean, low-emission, quiet, reliable, fuel adaptable, and highly efficient way to obtain power. An outstanding challenge in the design of SOFCs is that they must catalyze the oxygen reduction reaction, $O_2(gas) + 2e^- \rightarrow 2O^{2-}$ (solid). This reaction requires good catalysts and at present can only be done efficiently at high temperature, limiting the durability and applicability of the fuel cells. Today's SOFC catalysts are typically perovskite oxides, which can reduce O_2 gas and transport O^{2-} through their bulk to the electrolyte. I will discuss how quantum mechanical simulation methods can be used to understand catalytic mechanisms in cathodes and to discover superior perovskite cathode materials. In particular, I will demonstrate the use of the Oxygen 2p band center as a descriptor for materials performance and how it can be used to screen for highly catalytically active cathode materials. I will also present our development of a full molecular model of the surface catalytic processes, which model suggests a surprising role for surface termination and segregation. Overall our studies suggest that molecular simulation based prediction of the catalytic rates on perovskite SOFC cathodes may soon be possible.

Refreshments will be served before the seminar.
Please contact Tony Pulsone at pulsone@mit.edu with any questions.

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