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Transport in and chemistry on transition metal oxides for energy conversion

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We use quantum mechanics techniques to search for robust, efficient, and inexpensive materials for solid oxide fuel cells (SOFCs) that convert fuels to electricity, photovoltaics (PVs) that convert sunlight to electricity, and photo-catalytic electrodes (PCEs) that convert sunlight, CO_2, and H_2O into fuels. In our SOFC research, we focus on cathode optimization, often considered the limiting factor. If oxide ion diffusion and electron transport can be enhanced, along with rapid dissociative adsorption of dioxygen, lower temperatures can be used, which would facilitate wider deployment. In the solar energy conversion arena, the cost-efficiency tradeoff for PV materials motivates new options. I will discuss why it is difficult to find effective PCE materials; in particular I will enumerate the very significant constraints beyond those on PVs that they must satisfy to achieve high efficiency. Limiting oneself to abundant elements further constrains the design space. As a result, we are focusing primarily on first row transition metal oxide materials. Key properties of conventional and novel materials, along with some new design principles, will be discussed. The work is revealing which dopants or mixed oxides are likely to provide the most efficient energy conversion materials.