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Proton Diffusion Model for High-Throughput Calculations PANDU WISESA, TIM MUELLER, Department of Materials Science and Engineering, Johns Hopkins University — Solid oxide fuel cells (SOFCs) have many advantages over other fuel cells with high efficiency, myriad fuel choices, and low cost. The main issue however is the high operating temperature of SOFCs, which can be lowered by using an electrolyte material with high ionic conductivity, such as proton conducting oxides. Our goal is to identify promising proton-conducting materials in a manner that is time and cost efficient through the utilization of high-throughput calculations. We present a model for proton diffusion developed using machine learning techniques with training data that consists of density functional theory (DFT) calculations on various metal oxides. The built model is tested against other DFT results to see how it performs. The results of the DFT calculations and how the model fares are discussed, with focus on hydrogen diffusion pathways inside the bulk material.

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