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The effects of dopants on oxygen vacancies at grain boundaries in Ceria CeO_2

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The transport of ions or molecules through materials or at surfaces uniquely defines the reactivity and performance of many materials. For example, the operating temperature of Solid Oxide Fuel Cells (SOFC) is strongly correlated to the migration of oxygen ions through a bulk oxide material. For this reason, much research has been focused on finding ways to alter such pathways in key SOFC materials like ZrO_2 and CeO_2 [1,2]. Recent theory has demonstrated that migration barriers could be tuned through strain; tensile strain reduces migration barriers, and compressive strain increases said barriers. Similarly, migration barriers have been shown to be directly linked to the presence of dopants in bulk materials: again, larger dopants (which locally increase loacl volume) result in higher migration barriers, and smaller dopants result in dramatic reductions in these barriers [3–5].

Our work takes CeO_2 as case study for the systematic impact of different dopants on oxygen formation and migration pathways. Specific factors we address are the size of the dopant as well as its proximity to a twin boundary.

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