Computing the Fukui Function in Solid-State Chemistry: Application to Alkaline Earth Oxides Bulk and Surfaces

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Fukui functions (FFs) are chemical descriptors that are useful to explain the reactivity of systems toward electron transfer. Whereas they have been widely employed for molecules, their application to extended systems is scarce. One of the reasons for the limited development of such analysis in solids is the improper evaluation of FFs in the usual computational approaches based on density functional theory and periodic boundary conditions. In this work we compare the available approaches and propose a new method based on the interpolation of partially charged systems that mitigates some of the problems encountered. We discuss the reactivity of alkaline earth oxides (MgO, CaO, SrO, and BaO) in terms of the FF analysis, providing a robust way to account for the higher reactivity of surface oxygen sites compared with bulk sites.