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Electronic and energetics properties of oxygen defects in La2-xSrxCuO4 in relation to doping and strain[1] SOHEE PARK, Oak Ridge National Laboratory, CHANGWON PARK, University of Tennessee, MINA YOON[2], Oak Ridge National Laboratory — The level of oxygen defects in La2-xSrxCuO4 (LSCO), a high temperature superconductor, is known to drastically change LSCOs structural and electronic properties. However, the atomistic understanding of the role of oxygen defects is far from being complete. Using first-principles calculations, we investigated the electronic and energetic properties of oxygen vacancies in LSCO in relation to external parameters such as degree of Sr doping amount and external strain. We find that the relative stabilities between the equatorial vacancy induced in the CuO2 layer and the apical vacancy in the LaO layer can be altered by strain. In addition, Sr doping plays a crucial role in their relative stabilities. Therefore, the complex interplay between those key parameters essentially determines the overall oxygen density. Our finding can be instrumental in the experimental development of LSCO with desired oxygen density.

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