supporting information (SI)

Origins of Intrinsic p-type Conductivity, p-n Transition and Substoichiometry in SrO

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1. Energies curves as a function of the Sr-Sr bond length

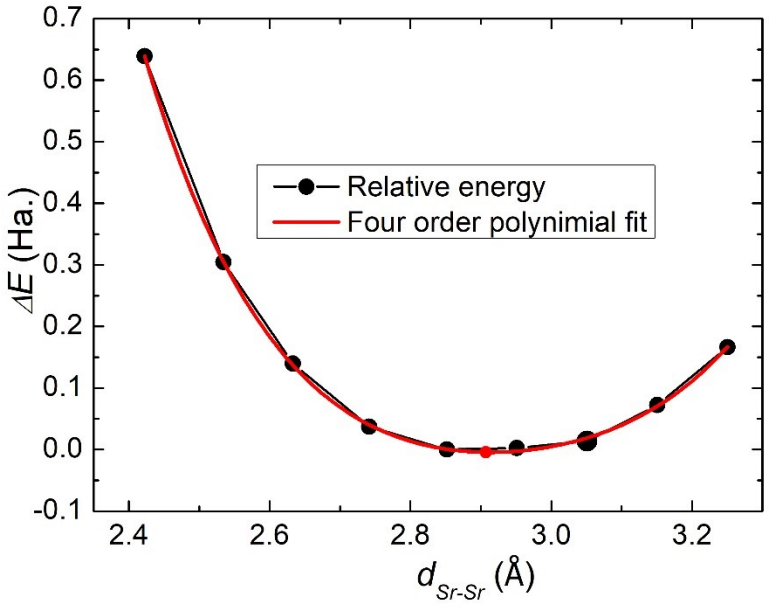

Figure S1. The energy curve as a function of the Sr-Sr bond length, and the red line is fitted with a fourth-order polynomial.

2. Formation energies of all defects at VBM

Table S3. The data of formation energies of V_o, V_{Sr}, O_i, and Sr_i under oxygen rich conditions at the VBM. For oxygen poor conditions, the difference is the SrO formation enthalpy which we take -6.182 eV[1]. Using these data, one can repeat the Figure 1 and 3 in the main text.

Defects	Charge	Oxygen rich		Oxygen poor	
		PBE0	BB1K	PBE0	BB1K
V_o	+2	-0.73153419	-0.58478943	-6.182	
	+1	2.129556934	2.262364999		
	0 ↑ ↑	7.983211073	8.209178628		
	0 ↑ ↓	6.525667362	6.445244413		
	−1 ↑ ↑	16.79394583	17.25901131		
	−1 ↑ ↓	15.58615147	15.63017921		
V_{Sr}	-2	5.201885784	5.674392243	+6.182	
	-1	3.689979208	4.03301462		
	0	2.42133562	2.661055248		
	+1	1.311229407	1.400374611		
	+2	0.429153163	0.369767893		
O_i	-2	8.408982115	8.607281794	+6.182	
	-1	4.973268892	5.231508931		
	0 ↑ ↑	2.871824832	3.074755074		
	0 ↑ ↓	0.62700147	0.665963527		
	+1	1.288870464	1.470439026		
Sr_i	+2	3.752012652	3.866544523	-6.182	
	+1	9.007137047	9.15382176		
	0	14.84527905	14.95443658		
	-1	20.76637337	20.91478002		

References：

1. I. J. Brink and C. E. Holley, *The Journal of Chemical Thermodynamics*, 1978, **10**, 259-266.