

Supporting information for Tailoring Lanthanide Doping in Perovskite CaTiO_3 for Luminescence Applications

Pei Yang,^{1,2} Bo Tai,³ Weikang Wu,³ Jian-Min Zhang,^{4,5} Feng Wang⁶, Shan Guan,¹
Wei Guo,¹ Yunhao Lu,⁷ and Shengyuan A. Yang,³

¹Beijing Key Laboratory of Nanophotonics and Ultrafine Optoelectronic Systems, School of Physics,
Beijing Institute of Technology, Beijing 100081, China

²Chinese Academy of Engineering Physics, Mianyang 621900, China

³Research Laboratory for Quantum Materials, Singapore University of Technology and Design,
Singapore 487372, Singapore

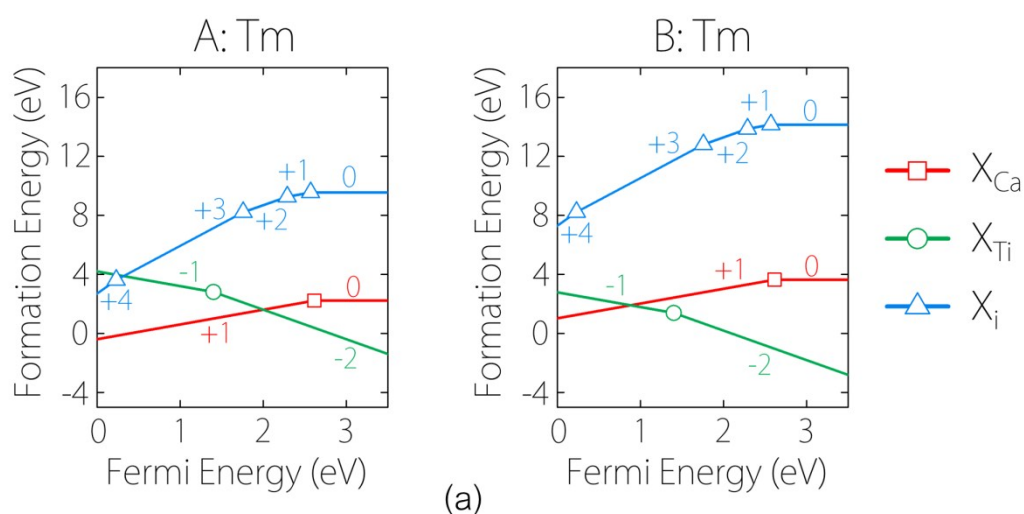
⁴College of Physics and Energy, Fujian Normal University, Fuzhou 350117, China

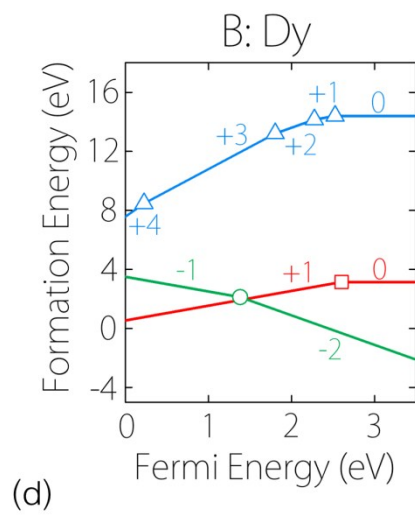
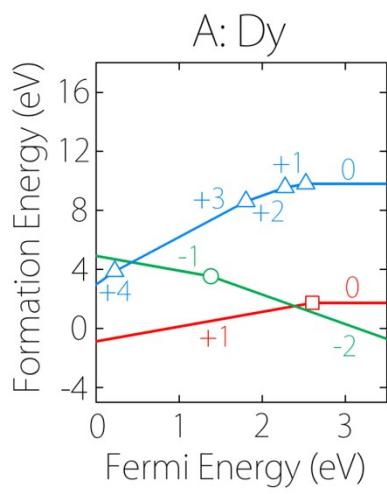
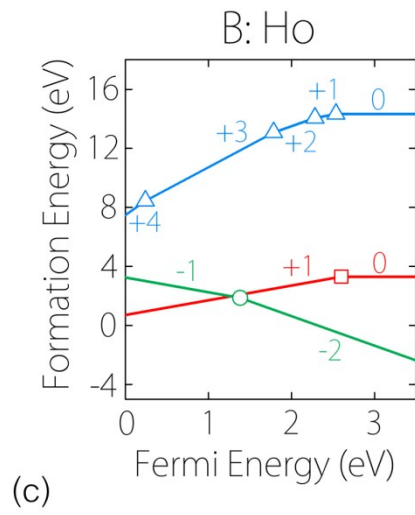
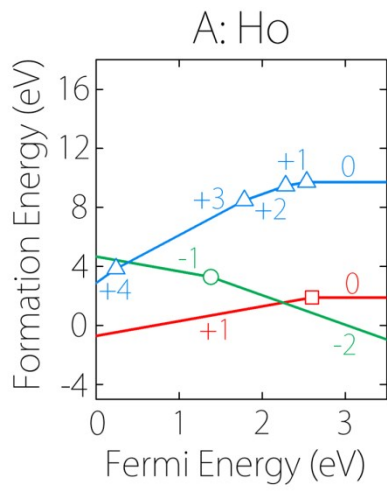
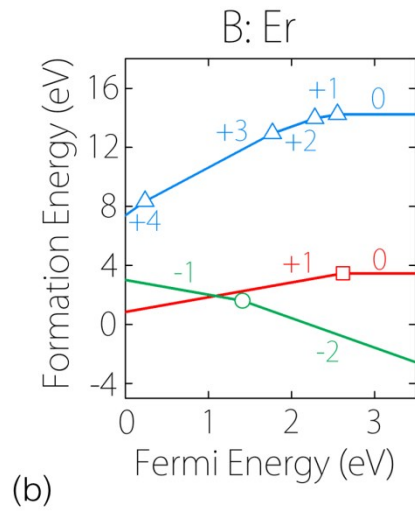
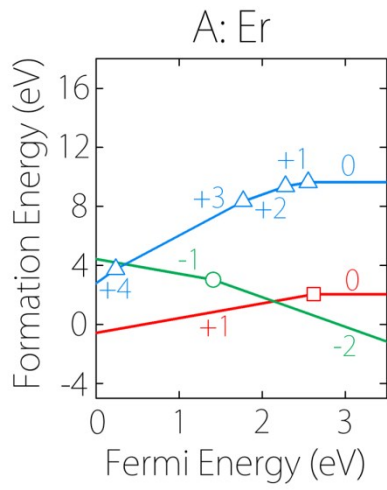
⁵Fujian Provincial Key Laboratory of Quantum Manipulation and New Energy Materials, Fuzhou
350117, China

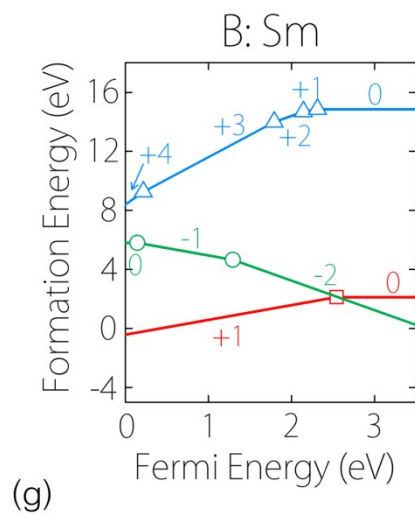
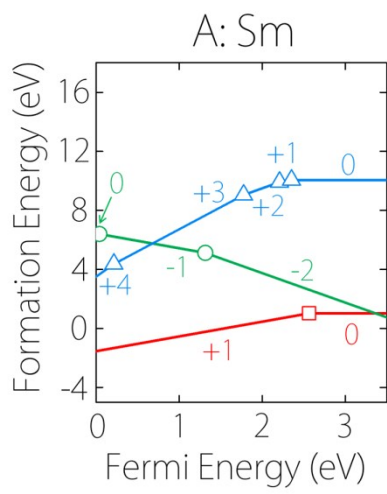
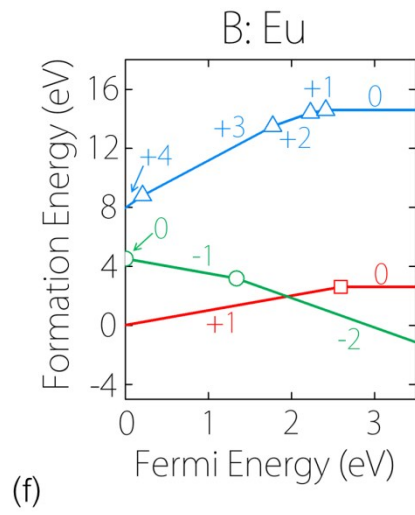
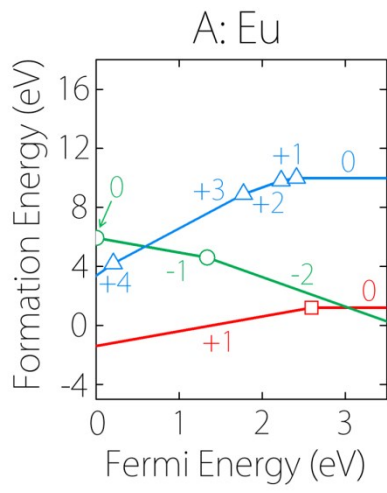
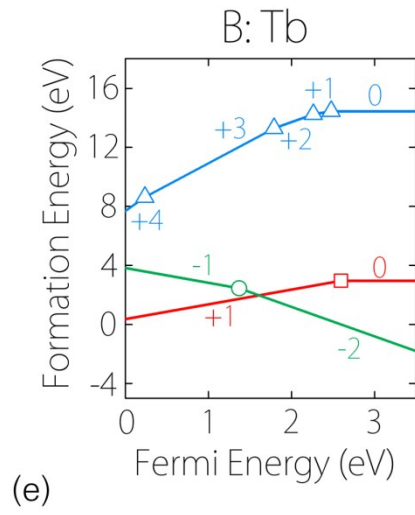
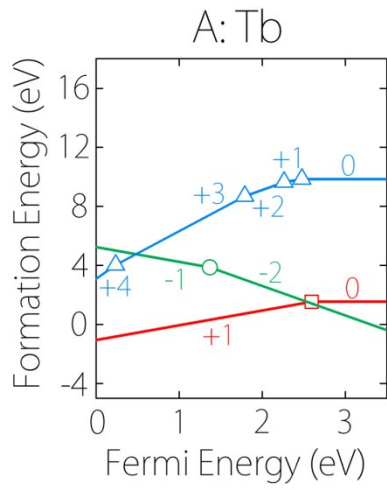
⁶Department of Physics and Materials Science, City University of Hong Kong, Hong Kong 999077,
China

⁷School of Materials Science and Engineering, Zhejiang University, Zhejiang 310027, China

We investigate doping of 11 rare-earth elements and determine the formation energies for various doping configurations. The results for Pr and Yb are discussed in the main text. Here we show the results for the remaining elements.







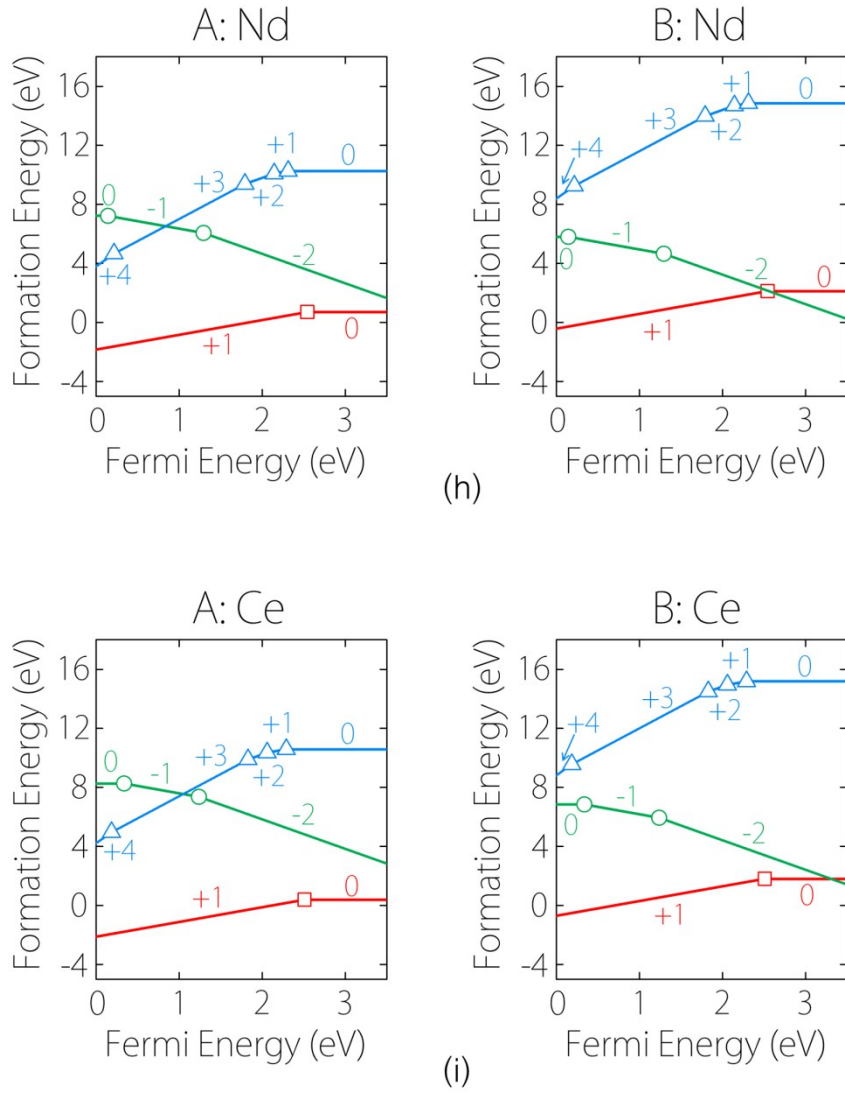


FIG. S1. Formation energies for (a) Tm, (b) Er, (c) Ho, (d) Dy, (e) Tb, (f) Eu, (g) Sm, (h) Nd and (i) Ce. Here A and B denote the “A point” (O-poor condition) and “B point” (O-rich condition) respectively. The red, green and blue line corresponds to different doping sites X_{Ca} , X_{Ti} and X_i , respectively (X =Tm, Er, Ho, Dy, Tb, Eu, Sm, Nd, Ce).