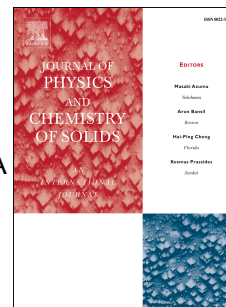


Accepted Manuscript

Revealing the doping mechanism and effect of cobalt on the HTB-type iron fluoride: A first-principle study

Zhijuan Zhang, Zhenhua Yang, Yang Li, Xianyou Wang



PII: S0022-3697(18)31561-0

DOI: [10.1016/j.jpcs.2018.07.001](https://doi.org/10.1016/j.jpcs.2018.07.001)

Reference: PCS 8655

To appear in: *Journal of Physics and Chemistry of Solids*

Received Date: 9 June 2018

Revised Date: 2 July 2018

Accepted Date: 8 July 2018

Please cite this article as: Z. Zhang, Z. Yang, Y. Li, X. Wang, Revealing the doping mechanism and effect of cobalt on the HTB-type iron fluoride: A first-principle study, *Journal of Physics and Chemistry of Solids* (2018), doi: 10.1016/j.jpcs.2018.07.001.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Revealing the doping mechanism and effect of cobalt on the HTB-type iron fluoride: A first-principle study

Zhijuan Zhang^{a,b}, Zhenhua Yang^{a,b,*}, Yang Li^{a,b}, Xianyou Wang^c

^aKey Laboratory of Materials Design and Preparation Technology of Hunan Province, School of Materials Science and Engineering, Xiangtan University, Xiangtan 411105, Hunan, China.

^bKey Laboratory of Low Dimensional Materials & Application Technology (Ministry of Education), School of Materials Science and Engineering, Xiangtan University, Xiangtan 411105, Hunan, China

^cSchool of Chemistry, Xiangtan University, Xiangtan 411105, Hunan, China

*Corresponding authors.

E-mail addresses: yangzhenhua@xtu.edu.cn (Zhenhua Yang)

Abstract

FeF₃ with a hexagonal-tungsten-bronze structure (HTB-FeF₃) has been proposed as a promising cathode material with high theoretical specific capacity and voltage. However, it suffers from the drawbacks of poor Li kinetics and cycling life due to poor electrical conductivity. Moreover, its fundamental information, such as its geometrical structure, elastic properties and electronic structure, can rarely be found. Hence, first-principle calculations have been carried out to systematically investigate the effects of Co doping on the FeF₃. We focus on Co_xFe_{1-x}F₃ systems, in which x is

Download English Version:

<https://daneshyari.com/en/article/7919798>

Download Persian Version:

<https://daneshyari.com/article/7919798>

[Daneshyari.com](https://daneshyari.com)