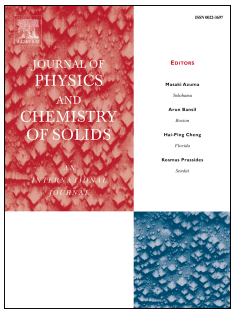
Accepted Manuscript



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

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.

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]

[a]*Key Laboratory of Materials Design and Preparation Technology of Hunan Province, School of Materials Science and Engineering, Xiangtan University, Xiangtan 411105, Hunan, China.*

[b]*Key Laboratory of Low Dimensional Materials &Application Technology* (*Ministry of Education*), *School of Materials Science and Engineering, Xiangtan University, Xiangtan 411105, Hunan, China*

[c]*School of Chemistry, Xiangtan University, Xiangtan 411105, Hunan, China*

[*]**Corresponding authors.**

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

Abstract

FeF_3 with a hexagonal-tungsten-bronze structure (HTB-FeF_3) 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 FeF_3. We focus on $Co_xFe_{1-x}F_3$ systems, in which *x* is