

Supporting Information

High-pressure effects on the electronic properties and photoluminescence of Ag-doped CsCu_2I_3

Zan Dou^{1#}, Zihua Lin^{1#}, Rong Wang², Mengmeng Han³, Jianxu Ding⁴, Haoyu Wang¹, Xiaoguang Luo¹, Yingchun Cheng^{2*}, Nannan Han^{1*}

¹Frontiers Science Center for Flexible Electronics, Institute of Flexible Electronics (IFE), Northwestern Polytechnical University, 127 West Youyi Road, Xi'an 710072, China

²Key Laboratory of Flexible Electronics & Institute of Advanced Materials, Jiangsu National Synergetic Innovation Center for Advanced Materials, Nanjing Tech University, 30 South Puzhu Road, Nanjing 211816, China

³China Petroleum Engineering & Construction Corp. North China Company, Middle Jianshe Road, Renqiu 062552, China

⁴College of Materials Science and Engineering, Shandong University of Science and Technology, Qingdao266590, China

*Email: iamyccheng@njtech.edu.cn, iamnnhan@nwpu.edu.cn

#Z. D. and Z. L. contributed equally to this work.

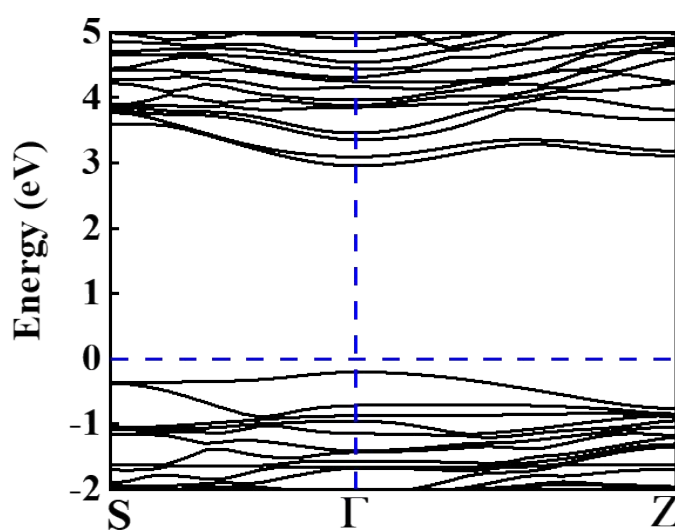


Figure S1. Band structure of the *cmcm* phase of 10% Ag doped CsCu_2I_3 at 7.5 GPa.

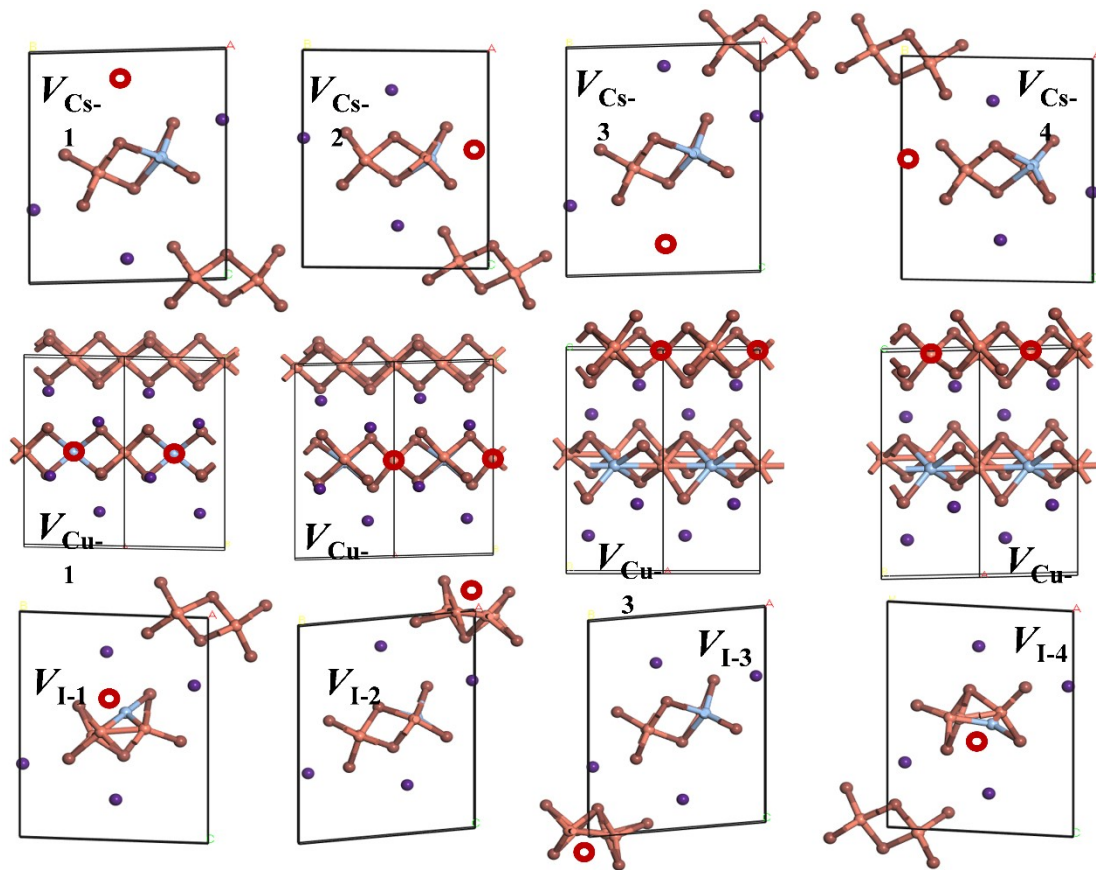


Figure S2. Structural diagram of the systems with vacancy defects. The circle shown is the location of the defects.

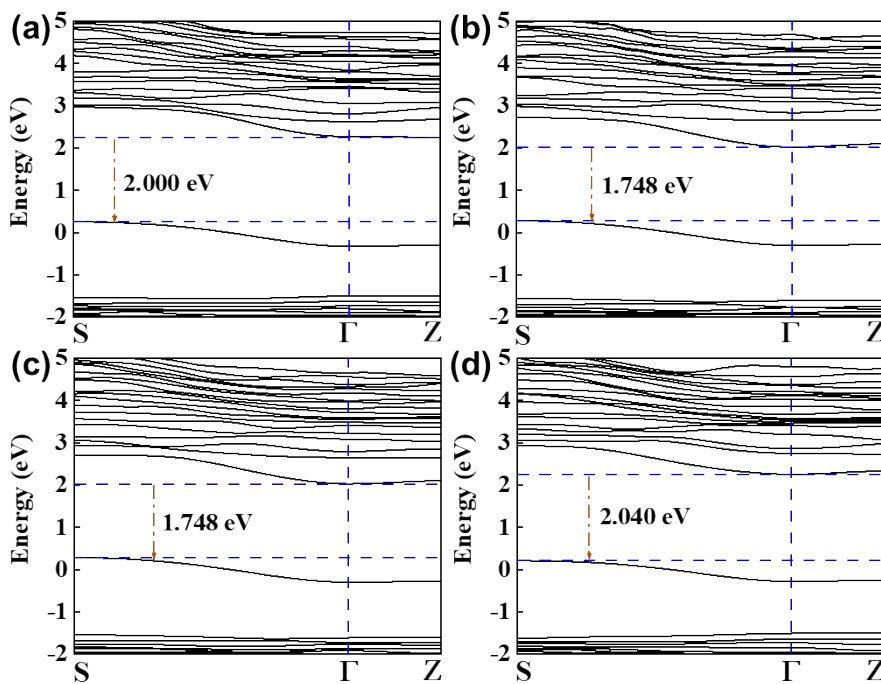


Figure S3. Band structure of 10% Ag doped CsCu_2I_3 system with four different

position I vacancies with position (a) 1, (b) 2, (c) 3, (d) 4.