Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Crystal structure of Cu_2Te predicted within adaptive genetic algorithm[1] KAI-MING HO, MANH CUONG NGUYEN, Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA, JINHO CHOI, ICQD, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui, 230026, China, CAI-ZHUANG WANG, XIN ZHAO, Ames Laboratory, US DOE and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA, ZHENYU ZHANG, ICQD, Hefei National Laboratory for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui, 230026, China — Cu_2Te is one of the most commonly used conductive back-contacting materials for high-efficiency CdTe-based solar cells. However, the detailed crystal structure of Cu_2Te is still undetermined blocking property investigations of the Cu_2Te-based solar cell systems. Some models have been proposed but all of them have positive formation energy [1]. We have performed adaptive genetic algorithm crystal structure search to find low energy crystal structures of Cu_2Te. We found a new layered-structure edged by Te atoms with negative formation energy from first-principles calculations within local density approximation. This layered structure consists of tilted Cu_2Te ribbon arrays. Structural and electronic properties of the newly found Cu_2Te structure will be discussed in detail.

[1] J. L. F. Da Silva, S.-H. Wei, J. Zhou, and X. Wu, Appl. Phys. Lett. 91, 091902 (2007)

[1]Supported in part US DOE, NSF of China, and US NSF.

Kai-Ming Ho
Ames Laboratory, US DOE and Dept of Physics and Astronomy,
Iowa State University, Ames, Iowa 50011, USA

Date submitted: 27 Nov 2012 Electronic form version 1.4