MRS-T 中國材料科學學會 Materials Research Society-Taiwan

Invited speaker's information form of IUMRS-ICA 2017

Presentation on Symposium F2:
Materials Design, Discovery, and Optimization Based on Computation

Presentation title: Topological Dirac nodal lines in pure metal beryllium and its potential applications

Speaker's name and affiliation: Xing-Qiu Chen (Institute of Metal Research, Chinese Academy of Sciences)

City/ Country: Shenyang, China

Email: xingqiu.chen@imr.ac.cn

Brief biography of Speaker:

Xing-Qiu Chen received his Ph.D degree in Physical Chemistry from the University of Vienna in 2004 and performed his postdoctoral studies at the Oak Ridge National Laboratory (ORNL). In 2010 he joined the Institute of Metal Research, Chinese Academy of Sciences funded by a CAS 'Hundred Talent Projects'. In 2015, he became Distinguished Professor of CAS Distinguished Research Fellow Program and in 2016 National Leading Talent of Young and Middle-aged Scientist Award from the Ministry of Science and Technology of China. He is a computational materials scientist, concerned with the computer modeling and algorithms of alloy properties and designs using quantum mechanical methodologies. To date, he has already published over 90 pre-review papers in scientific journals (including Nature Chem., 1 Nature Commun., Phys. Rev. Lett (9), Adv. Mater., and Phys. Rev. B (26)).

Abstract:

Beryllium is a simple alkali earth metal, but has been the target of intensive studies for decades because of its unusual electron behaviors at surfaces. Puzzling aspects include (i) severe deviations from the description of the nearly free electron picture, (ii) anomalously large electron-phonon coupling effect, and (iii) giant Friedel oscillations. The underlying origins for such anomalous surface electron behaviors have been under active debate, but with no consensus. Here, by means of first-principles calculations, we discover that this pure metal system, surprisingly, harbors the Dirac node line (DNL) that in turn helps to rationalize many of the existing puzzles. The DNL is featured by a closed line consisting of linear band crossings and its induced topological surface band agrees well with previous photoemission spectroscopy observation on Be (0001) surface. We further reveal that each of the elemental alkali earth metals of Mg, Ca, and Sr also harbors the DNL, and speculate that the fascinating topological property of DNL naturally exist in other elemental metals as well.

Please fill the above form and send it to Prof. Shih-kang Lin (linsk@mail.ncku.edu.tw), Prof. Nien-Ti Tsou (tsounienti@gmail.com), and Prof. Chih Chen (chih@mail.nctu.edu.tw).