Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Weak electron-phonon pairing in BiS2 superconductor from first principles RYOSUKE AKASHI, The University of Tokyo, Japan, CORENTIN MORICE[1], The University of Cambridge, United Kingdom, TAKASHI KORETSUNE, RIKEN Center for Emergent Matter Science, Japan, SIDDHARTH SAXENA, The University of Cambridge, United Kingdom, RYOTARO ARITA, RIKEN Center for Emergent Matter Science, Japan — The discovery of superconductivity in $Bi_4O_4S_3$, quickly followed by the one in La(O,F)BiS_2, opened up a new research field: novel BiS_2 superconductors. Many thorough experimental studies have been conducted but consensus on the nature of superconductivity in these materials has not been reached yet. One of the strongest pieces of evidence until now was the calculation of strong electron-phonon coupling in La(O,F)BiS_2 using ab-initio techniques, indicating that superconductivity in these materials is conventional and strongly coupled. Using density functional theory and the recently developed density functional theory for superconductors, we studied the possibility of phonon-mediated superconductivity. We first confirmed the arising of a commensurate charge density wave instability, in accordance with previous studies. Using a novel integration scheme for the electron-phonon coupling, we found that its strength is much lower than previously calculated, due to our improved convergence of density of state calculations. We finally conclude that the conventional phonon-mediated electron pairing cannot explain the high T_cs observed in this material.

[1]*Corresponding author cm712@cam.ac.uk

Ryosuke Akashi
The University of Tokyo

Date submitted: 11 Nov 2016 Electronic form version 1.4