Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPLEMENTARY INFORMATION

Superconductivity in $CaBi_2$

M.J. Winiarski[1,*], B. Wiendlocha[2], S. Gołąb[2], S. K. Kushwaha[3], P. Wisniewski[4], D. Kaczorowski[4], J. D. Thompson[5], R. J. Cava[3], T. Klimczuk[1,†]

[1] *Faculty of Applied Physics and Mathematics, Gdansk University of Technology, Narutowicza 11/12, 80-233 Gdansk, Poland*

[2] *Faculty of Physics and Applied Computer Science, AGH University of Science and Technology, Aleja Mickiewicza 30, 30-059 Krakow, Poland*

[3] *Department of Chemistry, Princeton University, Princeton NJ 08544, USA*

[4] *Institute for Low Temperature and Structure Research, Polish Academy of Sciences, PNr 1410, 50-950 Wrocław, Poland*

[5]*Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

* mwiniarski@mif.pg.gda.pl

† tomasz.klimczuk@pg.gda.pl

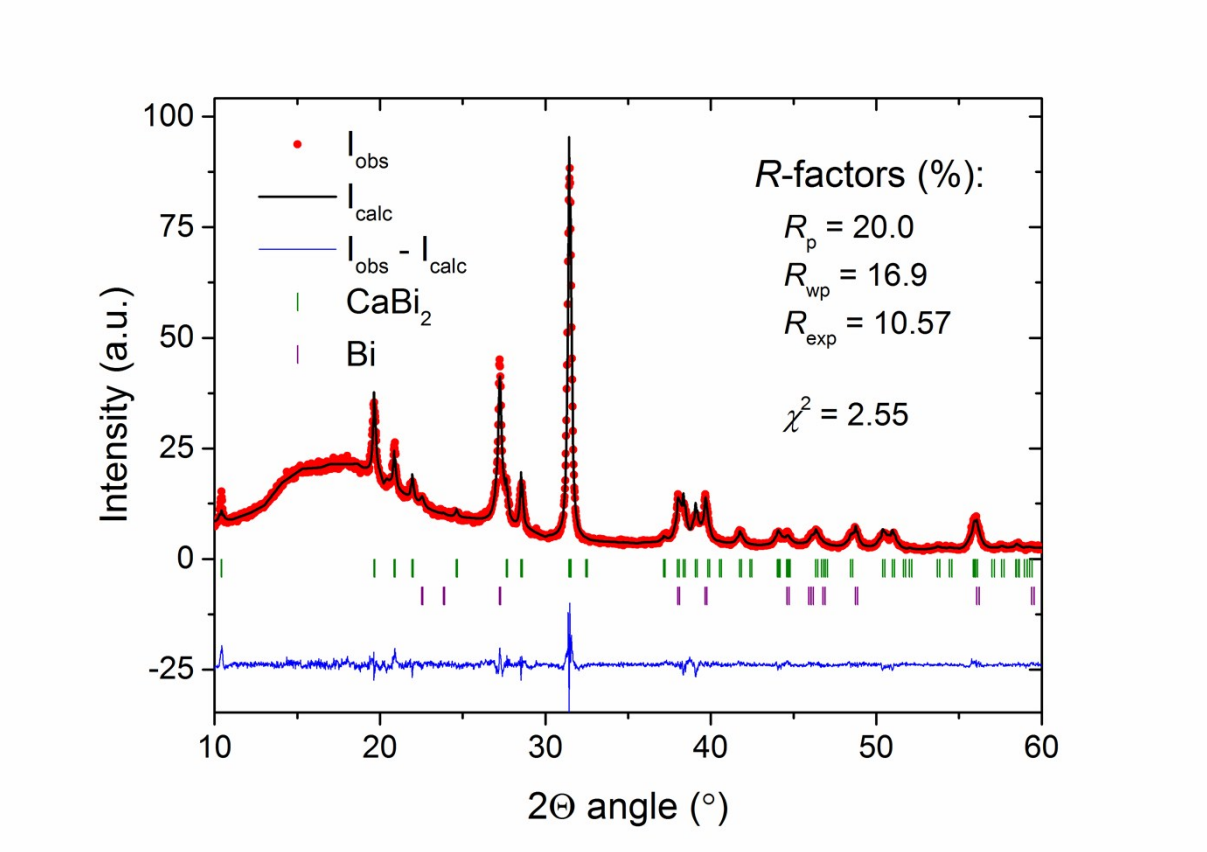

Fig. S1. Rietveld ($CaBi_2$ phase) and LeBail (Bi phase) fit to the diffraction pattern of ground $CaBi_2$ single crystals. Red points – observed intensities (I_{obs}), black solid line – calculated (I_{calc}), blue line – I_{obs}-I_{calc}, green and purple tics indicate the expected positions of Bragg reflections for $CaBi_2$ and Bi, respectively.

Table S1. Unit cell parameters and atomic positions obtained from a Rietveld fit (shown in Fig. S1). Values given in italics are repeated after Table 1 for comparison.

Unit cell parameters (Å):			
Rietveld refinement	4.6970(5)	17.069(2)	4.6127(4)
LeBail fit (see Tab. 1)	*4.696(1)*	*17.081(2)*	*4.611(1)*
Calculated (see Tab. 1)	*4.782*	*17.169*	*4.606*
Atomic positions:			
	x	*y*	*z*
Ca	0	0.0974(12)	¼
Bi(1)	0	0.4342(2)	¼
Bi(2)	0	0.7449(3)	¼
R-factors (%):			
R_p	R_{wp}	R_{exp}	χ^2
20.0	16.9	10.57	2.55

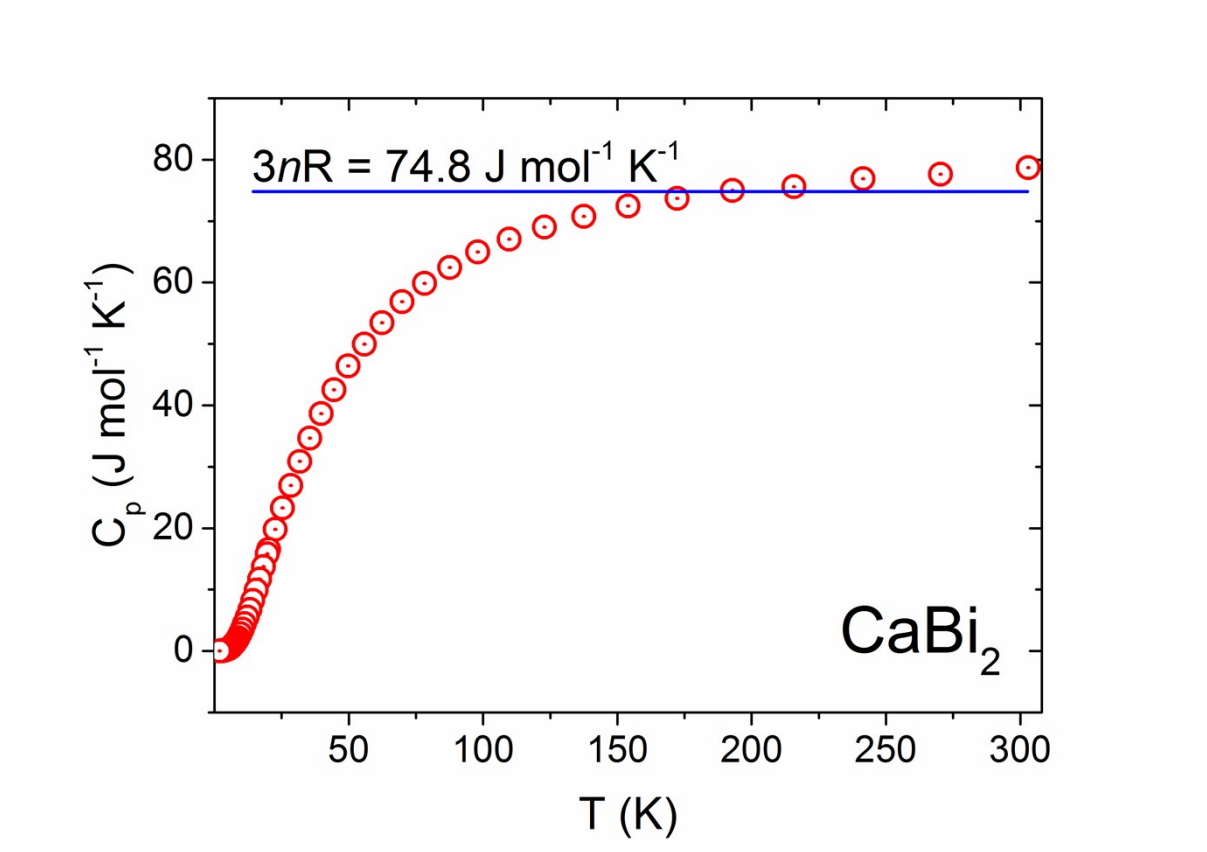

Fig. S2. Specific heat of $CaBi_2$ from 2 to 300 K. The solid blue line shows the value of specific heat calculated from the Dulong Petit Law assuming 3 atoms per formula unit.

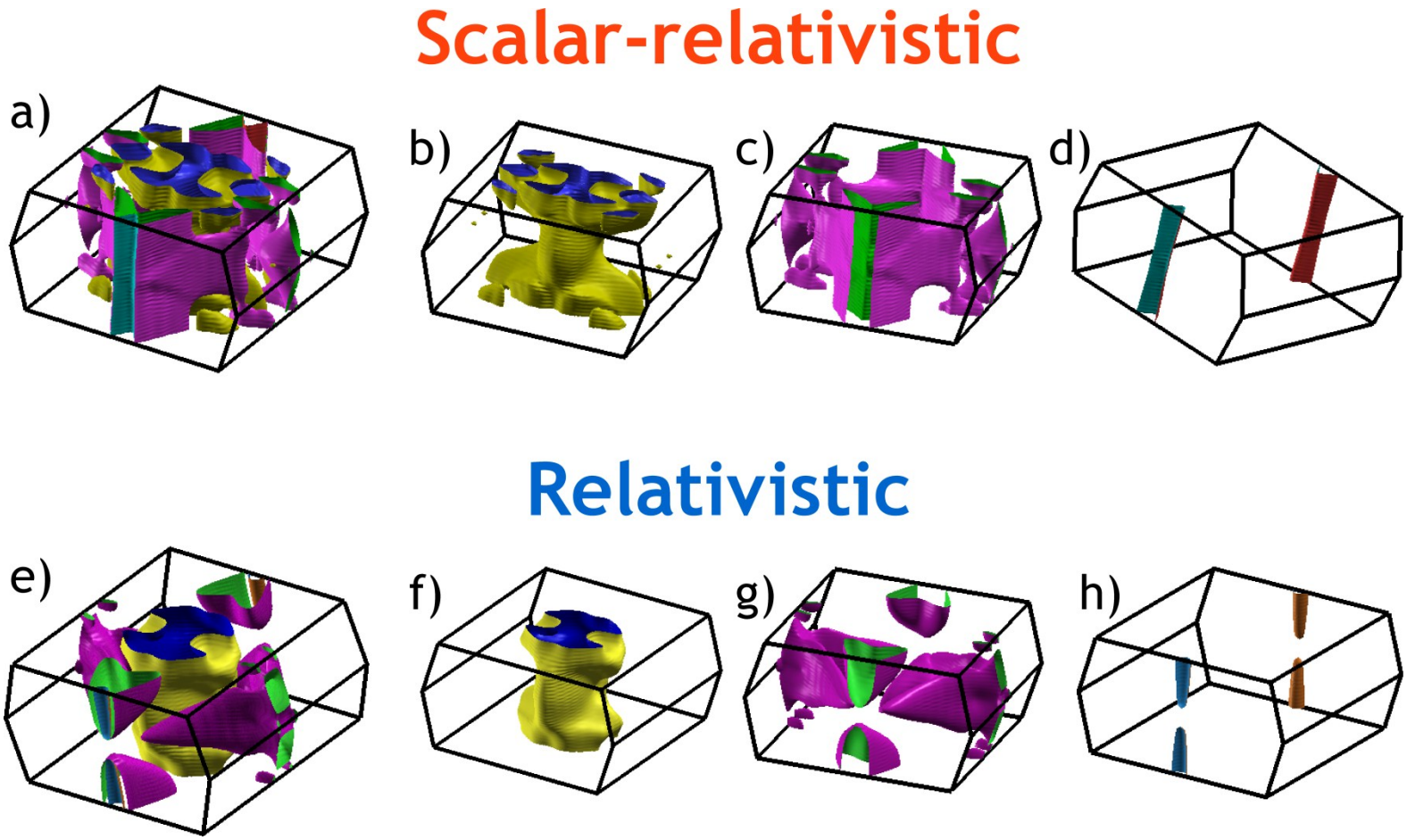

Fig. S3. The Fermi surface (FS) of $CaBi_2$: (a) scalar-relativistic case, (e) relativistic case; panels (b-d) and (f-h) show each of the three FS sheets in scalar-relativistic and relativistic case, respectively. Pictures prepared using XCrysDen [1].

[1] A. Kokalj, *J. Mol. Graph. Model*, 1999, **17**, 176. Code available from http://www.xcrysden.org/