Phase transition in CaFeAsH:

bridging 1111 and 122 iron-based superconductors

Yoshinori Muraba[†], *Soshi Iimura*[‡] *Satoru Matsuishi*[†], *Hidenori Hiramatsu*[‡]

Takashi Honda[§,¶], *Kazutaka Ikeda*[§,¶], *Toshiya Otomo*,[§,¶]*Hideo Hosono*[*,†,‡]

[†]Materials Research Center for Element Strategy, Tokyo Institute of Technology, 4259 Nagatsuta-cho, Midori-ku, Yokohama 226-8503, Japan

[‡]Materials and Structures Laboratory, Tokyo Institute of Technology, 4259 Nagatsuta-cho, Midori-ku, Yokohama 226-8503, Japan

[§] Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki 305-0801, Japan

[¶] J-PARC Center, KEK, Tokai, 319-1106, Japan

Corresponding author email: hosono@msl.titech.ac.jp

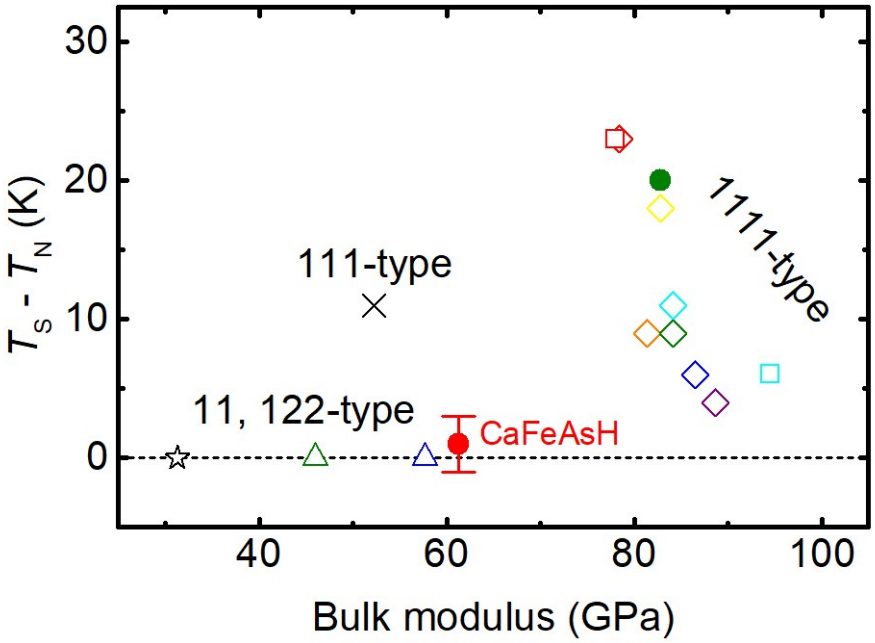

Figure S1: Plot of $T_s - T_N$ for various stoichiometric iron-based superconductors versus their bulk modulus. Red and green circles show experimental data of CaH- and CaF-1111, respectively.[1] Red and light blue diamonds are La- and Sm-1111, respectively.[2,3] Blue and green triangles are Ba- and Sr-122.[4,5] Black crosses and star are NaFeAs and FeTe, respectively.[6,7] The calculated data of La-, Ce-, Pr-, Nd-, Sm-, Tb-, and Gd-1111 are denoted by red, orange, yellow, green, light blue, blue, and purple squares, respectively.[8]

References

[1] H. Takahashi, T. Tomita, H. Soeda, M. Ebata, K. Okuma, T. Hanna, Y. Muraba, S. Matsuishi, and H. Hosono, J. Supercond. Nov. Magn. **25**, 1293 (2012).
[2] G. Garbarino, P. Toulemonde, M. Álvarez-Murga, A. Sow, M. Mezouar, and M. Núñez-Regueiro, Phys. Rev. B **78**, 100507 (2008).
[3] M. Calamiotou, D. Lampakis, E. Siranidi, J. Karpinski, N.D. Zhigadlo, and E. Liarokapis, Phys. C Supercond. **483**, 136 (2012).
[4] W. Uhoya, A. Stemshorn, G. Tsoi, Y.K. Vohra, A.S. Sefat, B.C. Sales, K.M. Hope, and S.T. Weir, Phys. Rev. B **82**, 144118 (2010).
[5] W.O. Uhoya, J.M. Montgomery, G.M. Tsoi, Y.K. Vohra, M.A. McGuire, A.S. Sefat, B.C. Sales, and S.T. Weir, J. Phys. Condens. Matter **23**, 122201 (2011).
[6] Q. Liu, X. Yu, X. Wang, Z. Deng, Y. Lv, J. Zhu, S. Zhang, H. Liu, W. Yang, L. Wang, H. Mao, G. Shen, Z.-Y. Lu, Y. Ren, Z. Chen, Z. Lin, Y. Zhao, and C. Jin, J. Am. Chem. Soc. **133**, 7892 (2011).
[7] C. Zhang, W. Yi, L. Sun, X.-J. Chen, R.J. Hemley, H. Mao, W. Lu, X. Dong, L. Bai, J. Liu, A.F. Moreira Dos Santos, J.J. Molaison, C.A. Tulk, G. Chen, N. Wang, and Z. Zhao, Phys. Rev. B **80**, 144519 (2009).
[8] H. Li, Z. Wu, S. Zhou, S. Zhang, X. Pu, S. Yao, X. Wang, and J. Yin, J. Alloys Compd. **632**, 303 (2015).