Supporting Information:

Multifunctional BBF Monolayer with High Mechanical Flexibility and Strong SHG response

Yilimiranmu Rouzhahong, Mamatrishat Mamat*, Baoxia Mu and Qian Wang

School of Physics and technology, Xinjiang University, 666 Victory Road, Urumqi 830046, China

S1. Bulk modulus and shear modulus

In this work , bulk modulus and shear modulus were calculated by using equation as given in S1 and S2: [1]

$$B = \frac{1}{2}\left\{[(2S_{11} + S_{33}) + 2(S_{12} + 2S_{13})]^{-1} + \left[\frac{1}{9}(2C_{11} + C_{33}) + \frac{2}{9}(C_{12} + 2C_{13})\right]\right\}, \quad \text{Eq. (S1)}$$

$$G = \frac{1}{2}\left\{15[4(2S_{11} + S_{33}) - 4(S_{12} + 2S_{13}) + 6(S_{44} + S_{11} - S_{12})]^{-1} + \left[\frac{1}{15}(2C_{11} + C_{33} - C_{12} - 2C_{13}) + \frac{1}{15}\left(2C_{44} + \frac{C_{11} - C_{12}}{2}\right)\right]\right\}. \quad \text{Eq.(S2)}$$

Where, the S_{ij} corresponds to the elastic compliance constants, calculated S_{ij} value is given in Table S1.

Table S1 Calculated elastic compliance constants

S_{11}	S_{12}	S_{13}	S_{14}	S_{15}	S_{33}	S_{44}
0.02	-0.006	-0.05	0.01	0.0	3.31	0.21

Table S2 Calculated Poisson's ratio

ν_{ab}	ν_{ba}	ν_{ac}	ν_{bc}	ν_{ca}	ν_{cb}
0.28	0.28	2.22	2.22	0.02	0.02

S2. Angular dependent Young's modul, and Poisson's ratio

In this work, angular dependent Young modul and Poisson's ratio were calculated by using equation as given in S3 and S4. [2]

Angular dependent Young modul :

$$\mathrm{Y}(\theta) = \frac{1}{\mu_1 + 2\mu_2 + \sin^4\theta\ \ \mu_3 + 2\sin^2\theta\ \ \mu_4 + 4\sin^2\theta\ \ \mu_5}\quad , \qquad \text{Eq.}\quad (S3)$$

Angular dependent Poisson's ratio

$$\nu(\theta) = \frac{\mu_1 + \sin^2\theta\cos^2\theta\ \ \mu_3/2 + (1-\cos^2\theta/2)/\mu_4}{\mu_1 + 2\mu_2 + \sin^4\theta\ \ \mu_3 + 2\sin^2\theta\ \ \mu_4 + 4\sin^2\theta\ \ \mu_5}\quad . \qquad \text{Eq.}\quad (S4)$$

where $\mu_1 = S_{12},\ \mu_2 = (S_{11} - S_{12})/2\ ,\mu_3 = S_{11} + S_{33} - 2S_{13} - S_{44},\ \ \mu_4 = S_{13} - S_{12},\ \ \ \mu_5 = (S_{44} - 2S_{11} + 2S_{12})/4$ and related S_{ij} value given in Table S2.

References

1. Q. J. Liu, H. Qin, Z. Jiao, F. S. Liu, and Z. T. Liu, Mater. Chem. Phys.,2016, **180** , 75.
2. R. Schuster, C. Habenicht, M. Ahmad, M. Knupfer, and B. BUchner, Phys. Rev. B, 2018, **97**, 041201.