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:\(^1\)

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

Eq. (S1)

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

Eq.(S2)

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

<table>
<thead>
<tr>
<th>( S_{11} )</th>
<th>( S_{12} )</th>
<th>( S_{13} )</th>
<th>( S_{14} )</th>
<th>( S_{15} )</th>
<th>( S_{33} )</th>
<th>( S_{44} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.02</td>
<td>-0.006</td>
<td>-0.05</td>
<td>0.01</td>
<td>0.0</td>
<td>3.31</td>
<td>0.21</td>
</tr>
</tbody>
</table>

Table S1 Calculated elastic compliance constants

<table>
<thead>
<tr>
<th>( \nu_{ab} )</th>
<th>( \nu_{ba} )</th>
<th>( \nu_{ac} )</th>
<th>( \nu_{bc} )</th>
<th>( \nu_{ca} )</th>
<th>( \nu_{cb} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.28</td>
<td>0.28</td>
<td>2.22</td>
<td>2.22</td>
<td>0.02</td>
<td>0.02</td>
</tr>
</tbody>
</table>

Table S2 Calculated Poisson’s ratio
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. 

Angular dependent Young modul :

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

Angular dependent Poisson’s ratio

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

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