**Supplementary Information**

**Machine Learning-Driven Prediction of the Glass Transition Temperature of Styrene-Butadiene Rubber**

*Zhanglei Wang1,2, Shuo Yan1,2*, *Jingyu Gao**1,2, Haoyu Wu1,2, Baili Wang1,2, Xiuying Zhao1,2\*, and Shikai Hu1,2\**

1 State Key Laboratory of Organic-Inorganic Composites, Beijing University of Chemical Technology, Beijing, 100029, China

2 Beijing Engineering Research Center of Advanced Elastomers, Beijing University of Chemical Technology, Beijing, 100029, China

\* Corresponding author:

zhaoxy@mail.buct.edu.cn (Xiuying Zhao)

skhu@mail.buct.edu.cn (Shikai Hu)

**Table S1:** Summary of SBR Structural Composition and Corresponding *Tg* Data

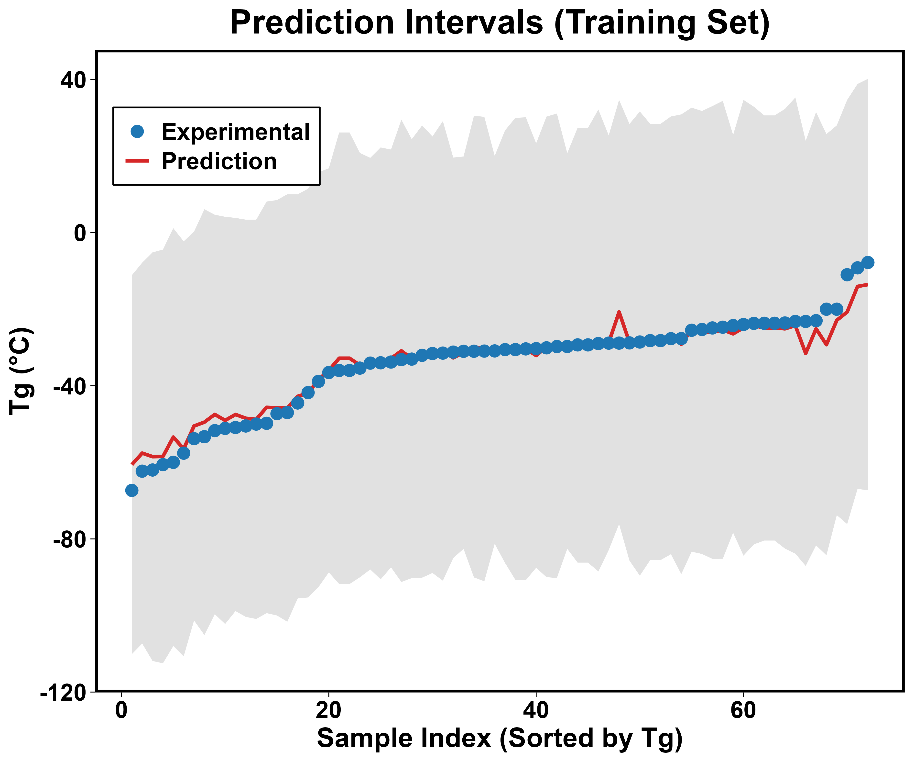
|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Sample number | Styrene/% | 1,2-butadiene/% | Cis-1, 4-butadiene/% | Trans-1, 4-butadiene/% | *T*g/℃ |
| 1 | 23.93 | 11.99 | 8.88 | 55.2 | -53.82 |
| 2 | 21.34 | 52.84 | 12.06 | 13.75 | -23.67 |
| 3 | 3.64 | 7.43 | 29.41 | 38.53 | -67.33 |
| 4 | 27.25 | 43.22 | 12.41 | 17.12 | -28.8 |
| 5 | 27.65 | 39.34 | 14.42 | 18.6 | -29.32 |
| 6 | 27.39 | 41.65 | 12.09 | 18.86 | -28.21 |
| 7 | 23.5 | 19.5 | 12 | 68 | -60 |
| 8 | 25 | 26 | 26 | 48 | -50 |
| 9 | 21.1 | 35.5 | 14.4 | 50.2 | -51.72 |
| 10 | 26.3 | 35 | 12.7 | 52.3 | -47.29 |
| 11 | 35.3 | 35.1 | 10.4 | 54.5 | -38.86 |
| 12 | 31.1 | 34.5 | 12 | 53.5 | -41.78 |
| 13 | 34.8 | 30 | 13.5 | 56.4 | -44.49 |
| 14 | 35.9 | 40.5 | 9.6 | 49.9 | -31.21 |
| 15 | 30.6 | 41.3 | 10.2 | 48.6 | -35.9 |
| 16 | 23 | 12.2 | 10.7 | 54.1 | -59.15 |
| 17 | 23.7 | 12.6 | 10.5 | 53.2 | -56.53 |
| 18 | 39.9 | 9.3 | 12.5 | 38.3 | -40.28 |
| 19 | 22.4 | 45.8 | 10.5 | 21.3 | -30.56 |
| 20 | 22.9 | 48.4 | 11.4 | 17.3 | -33.8 |
| 21 | 26.9 | 64.1 | 17.8 | 18 | -22 |
| 22 | 27.2 | 59.2 | 18.9 | 21.9 | -25.3 |
| 23 | 26.4 | 63.3 | 18 | 18.8 | -23.7 |
| 24 | 22.3 | 61.6 | 18.4 | 20 | -25.5 |
| 25 | 23.5 | 60.9 | 17.9 | 21.2 | -23.2 |
| 26 | 23.5 | 60.5 | 17.2 | 22.3 | -24.7 |
| 27 | 23.5 | 58.7 | 19.1 | 22.2 | -24.9 |
| 28 | 23.5 | 51.6 | 21.9 | 26.4 | -30.3 |
| 29 | 25 | 58.7 | 14.9 | 26.3 | -23.6 |
| 30 | 25 | 11.3 | 37.3 | 52.5 | -57.6 |
| 31 | 17 | 12.5 | 37.4 | 50.1 | -62.3 |
| 32 | 26 | 11.6 | 39.1 | 49.3 | -62 |
| 33 | 23.5 | 18.7 | 19.4 | 61.8 | -49.8 |
| 34 | 25 | 63 | 15.2 | 21.8 | -4.7 |
| 35 | 21 | 68 | 17 | 15 | -7.8 |
| 36 | 26.2 | 58 | 19.7 | 22.3 | -36 |
| 37 | 23.5 | 31.1 | 16.2 | 52.7 | -20 |
| 38 | 23 | 53.6 | 17.3 | 29.1 | -34 |
| 39 | 21 | 18.7 | 19.8 | 61.5 | -50.9 |
| 40 | 25 | 32.1 | 26.7 | 41.2 | -50.5 |
| 41 | 23 | 47.4 | 20.8 | 31.7 | -49.8 |
| 42 | 25 | 13.5 | 35.8 | 50.6 | -60.6 |
| 43 | 25 | 13.5 | 37 | 49.4 | -61.3 |
| 44 | 23.5 | 20.6 | 13.9 | 65.6 | -47 |
| 45 | 23 | 20.8 | 13.1 | 66.1 | -23.2 |
| 46 | 21.34 | 52.84 | 12.06 | 13.75 | -23.67 |
| 47 | 24.64 | 7.43 | 29.41 | 38.53 | -67.33 |
| 48 | 27.25 | 43.22 | 12.41 | 17.12 | -28.8 |
| 49 | 27.65 | 39.34 | 14.42 | 18.6 | -29.32 |
| 50 | 27.39 | 41.65 | 12.09 | 18.86 | -28.21 |
| 51 | 24.9 | 59 | 19.4 | 21.6 | -26.71 |
| 52 | 35.1 | 50.9 | 22.7 | 26.4 | -22.36 |
| 53 | 36.6 | 40.4 | 26.7 | 32.9 | -30.9 |
| 54 | 22.9 | 48.4 | 11.4 | 17.3 | -30.56 |
| 55 | 22.4 | 45.8 | 10.5 | 21.3 | -33.8 |
| 56 | 26.2 | 58 | 19.7 | 22.3 | -36 |
| 57 | 27.7 | 58 | 20.6 | 21.4 | -23 |
| 58 | 25.2 | 59 | 18.7 | 19.6 | -24 |
| 59 | 34.5 | 50.1 | 23.8 | 26.1 | -20 |
| 60 | 13.8 | 59.9 | 19.4 | 22.7 | -31 |
| 61 | 25.6 | 36.5 | 23.1 | 14.8 | -26.64 |
| 62 | 26.4 | 35.9 | 23.1 | 14.6 | -24.28 |
| 63 | 25.5 | 41.2 | 19.5 | 13.8 | -28.86 |
| 64 | 22.1 | 61.5 | 21.3 | 17.2 | -28.5 |
| 65 | 25.4 | 62.5 | 20.1 | 17.4 | -27.7 |
| 66 | 19.36 | 61.85 | 12.57 | 25.57 | -27.68 |
| 67 | 20.12 | 62.54 | 13.22 | 24.23 | -29.24 |
| 68 | 20.56 | 61.58 | 13.36 | 25.06 | -30.94 |
| 69 | 21.75 | 63.13 | 13.32 | 23.56 | -28.97 |
| 70 | 16.52 | 61.52 | 13.89 | 24.59 | -31.58 |
| 71 | 15.62 | 62.14 | 12.56 | 25.29 | -35.38 |
| 72 | 16.75 | 61.85 | 13.05 | 25.1 | -33.03 |
| 73 | 20.16 | 62.85 | 12.63 | 24.51 | -28.57 |
| 74 | 21.55 | 63.12 | 11.99 | 24.89 | -28.46 |
| 75 | 19.85 | 62.59 | 12.47 | 24.94 | -30.37 |
| 76 | 20.56 | 62.85 | 12.49 | 24.65 | -29.75 |
| 77 | 21.56 | 62.99 | 12.35 | 24.66 | -30.98 |
| 78 | 21.54 | 62.41 | 12.56 | 25.02 | -28.28 |
| 79 | 19.85 | 61.58 | 13.65 | 24.76 | -30.55 |
| 80 | 20.98 | 62.45 | 11.89 | 25.65 | -30.09 |
| 81 | 20.79 | 63.54 | 10.86 | 25.6 | -32.04 |
| 82 | 20.56 | 62.98 | 12.87 | 24.15 | -31.19 |
| 83 | 21.57 | 63.2 | 11.96 | 24.85 | -30.95 |
| 84 | 19.85 | 63.53 | 11.95 | 24.61 | -31.47 |
| 85 | 21.85 | 62.55 | 13.05 | 24.4 | -33.17 |
| 86 | 27.2 | 68.7 | 6.5 | 31.9 | -20.78 |
| 87 | 25.8 | 65 | 8.3 | 26.7 | -28.85 |
| 88 | 27.2 | 62.7 | 6.5 | 31.9 | -9.2 |
| 89 | 25.8 | 65 | 8.3 | 26.7 | -11 |
| 90 | 34.4 | 25 | 40.6 | 34.4 | -34.08 |
| 91 | 37.1 | 25.2 | 37.7 | 37.1 | -29.74 |
| 92 | 33.6 | 24.1 | 42.3 | 33.6 | -36.54 |
| 93 | 36.4 | 24.9 | 38.7 | 36.4 | -31.99 |
| 94 | 27.5 | 24.4 | 14.9 | 60.7 | -51.13 |
| 95 | 25.5 | 39.4 | 12 | 48.6 | -46.94 |
| 96 | 25.6 | 32.1 | 14.5 | 53.4 | -53.31 |

**Table S2:** The summary of the actual Tg and the predicted Tg values corresponding to different SBR structural compositions in the training set

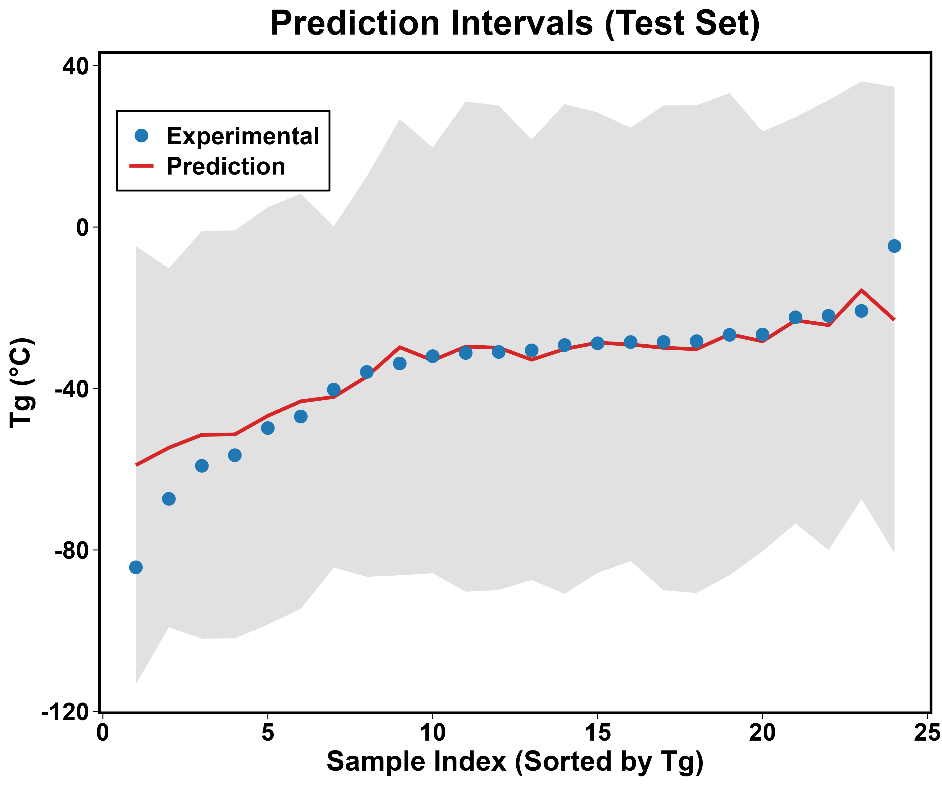
|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Sample number | Styrene/% | 1,2-butadiene/% | Cis-1, 4-butadiene/% | Trans-1, 4-butadiene/% | *T*g/℃ | Predicted *T*g/℃ |
| 1 | 23.93 | 11.99 | 8.88 | 55.2 | -53.82 | -50.51 |
| 2 | 21.34 | 52.84 | 12.06 | 13.75 | -23.67 | -24.90 |
| 3 | 3.64 | 7.43 | 29.41 | 38.53 | -67.33 | -60.62 |
| 4 | 27.25 | 43.22 | 12.41 | 17.12 | -28.8 | -28.65 |
| 5 | 27.65 | 39.34 | 14.42 | 18.6 | -29.32 | -29.41 |
| 6 | 27.39 | 41.65 | 12.09 | 18.86 | -28.21 | -28.56 |
| 7 | 23.5 | 19.5 | 12 | 68 | -60 | -53.41 |
| 8 | 25 | 26 | 26 | 48 | -50 | -48.76 |
| 9 | 21.1 | 35.5 | 14.4 | 50.2 | -51.72 | -47.49 |
| 10 | 26.3 | 35 | 12.7 | 52.3 | -47.29 | -45.75 |
| 11 | 35.3 | 35.1 | 10.4 | 54.5 | -38.86 | -38.41 |
| 12 | 31.1 | 34.5 | 12 | 53.5 | -41.78 | -41.92 |
| 13 | 34.8 | 30 | 13.5 | 56.4 | -44.49 | -42.76 |
| 14 | 35.9 | 40.5 | 9.6 | 49.9 | -31.21 | -32.70 |
| 15 | 27.2 | 59.2 | 18.9 | 21.9 | -25.3 | -26.08 |
| 16 | 26.4 | 63.3 | 18 | 18.8 | -23.7 | -24.27 |
| 17 | 22.3 | 61.6 | 18.4 | 20 | -25.5 | -25.34 |
| 18 | 23.5 | 60.9 | 17.9 | 21.2 | -23.2 | -24.27 |
| 19 | 23.5 | 60.5 | 17.2 | 22.3 | -24.7 | -25.38 |
| 20 | 23.5 | 58.7 | 19.1 | 22.2 | -24.9 | -26.07 |
| 21 | 23.5 | 51.6 | 21.9 | 26.4 | -30.3 | -32.11 |
| 22 | 25 | 58.7 | 14.9 | 26.3 | -23.6 | -25.11 |
| 23 | 25 | 11.3 | 37.3 | 52.5 | -57.6 | -56.48 |
| 24 | 17 | 12.5 | 37.4 | 50.1 | -62.3 | -57.59 |
| 25 | 26 | 11.6 | 39.1 | 49.3 | -62 | -58.52 |
| 26 | 21 | 68 | 17 | 15 | -7.8 | -13.56 |
| 27 | 26.2 | 58 | 19.7 | 22.3 | -36 | -32.81 |
| 28 | 23.5 | 31.1 | 16.2 | 52.7 | -20 | -29.26 |
| 29 | 23 | 53.6 | 17.3 | 29.1 | -34 | -34.15 |
| 30 | 21 | 18.7 | 19.8 | 61.5 | -50.9 | -47.50 |
| 31 | 25 | 32.1 | 26.7 | 41.2 | -50.5 | -48.50 |
| 32 | 23 | 47.4 | 20.8 | 31.7 | -49.8 | -45.63 |
| 33 | 25 | 13.5 | 35.8 | 50.6 | -60.6 | -58.45 |
| 34 | 23.5 | 20.6 | 13.9 | 65.6 | -47 | -45.80 |
| 35 | 23 | 20.8 | 13.1 | 66.1 | -23.2 | -31.54 |
| 36 | 21.34 | 52.84 | 12.06 | 13.75 | -23.67 | -24.90 |
| 37 | 27.65 | 39.34 | 14.42 | 18.6 | -29.32 | -29.41 |
| 38 | 27.39 | 41.65 | 12.09 | 18.86 | -28.21 | -28.56 |
| 39 | 36.6 | 40.4 | 26.7 | 32.9 | -30.9 | -30.62 |
| 40 | 22.9 | 48.4 | 11.4 | 17.3 | -30.56 | -29.78 |
| 41 | 22.4 | 45.8 | 10.5 | 21.3 | -33.8 | -32.86 |
| 42 | 26.2 | 58 | 19.7 | 22.3 | -36 | -32.81 |
| 43 | 27.7 | 58 | 20.6 | 21.4 | -23 | -25.11 |
| 44 | 25.2 | 59 | 18.7 | 19.6 | -24 | -24.85 |
| 45 | 34.5 | 50.1 | 23.8 | 26.1 | -20 | -22.89 |
| 46 | 13.8 | 59.9 | 19.4 | 22.7 | -31 | -31.35 |
| 47 | 26.4 | 35.9 | 23.1 | 14.6 | -24.28 | -26.44 |
| 48 | 25.5 | 41.2 | 19.5 | 13.8 | -28.86 | -28.76 |
| 49 | 25.4 | 62.5 | 20.1 | 17.4 | -27.7 | -26.83 |
| 50 | 19.36 | 61.85 | 12.57 | 25.57 | -27.68 | -29.15 |
| 51 | 20.56 | 61.58 | 13.36 | 25.06 | -30.94 | -30.41 |
| 52 | 21.75 | 63.13 | 13.32 | 23.56 | -28.97 | -28.17 |
| 53 | 16.52 | 61.52 | 13.89 | 24.59 | -31.58 | -31.89 |
| 54 | 15.62 | 62.14 | 12.56 | 25.29 | -35.38 | -34.61 |
| 55 | 16.75 | 61.85 | 13.05 | 25.1 | -33.03 | -32.92 |
| 56 | 20.16 | 62.85 | 12.63 | 24.51 | -28.57 | -28.98 |
| 57 | 19.85 | 62.59 | 12.47 | 24.94 | -30.37 | -30.33 |
| 58 | 20.56 | 62.85 | 12.49 | 24.65 | -29.75 | -29.54 |
| 59 | 21.56 | 62.99 | 12.35 | 24.66 | -30.98 | -29.77 |
| 60 | 19.85 | 61.58 | 13.65 | 24.76 | -30.55 | -30.36 |
| 61 | 20.98 | 62.45 | 11.89 | 25.65 | -30.09 | -29.85 |
| 62 | 20.79 | 63.54 | 10.86 | 25.6 | -32.04 | -31.06 |
| 63 | 19.85 | 63.53 | 11.95 | 24.61 | -31.47 | -30.89 |
| 64 | 21.85 | 62.55 | 13.05 | 24.4 | -33.17 | -30.88 |
| 65 | 25.8 | 65 | 8.3 | 26.7 | -28.85 | -20.73 |
| 66 | 27.2 | 62.7 | 6.5 | 31.9 | -9.2 | -14.05 |
| 67 | 25.8 | 65 | 8.3 | 26.7 | -11 | -20.73 |
| 68 | 34.4 | 25 | 40.6 | 34.4 | -34.08 | -34.22 |
| 69 | 37.1 | 25.2 | 37.7 | 37.1 | -29.74 | -30.92 |
| 70 | 33.6 | 24.1 | 42.3 | 33.6 | -36.54 | -35.97 |
| 71 | 27.5 | 24.4 | 14.9 | 60.7 | -51.13 | -49.04 |
| 72 | 25.6 | 32.1 | 14.5 | 53.4 | -53.31 | -49.50 |

**Table S3:** The summary of the actual Tg and the predicted Tg values corresponding to different SBR structural compositions in the test set

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Sample number | Styrene/% | 1,2-butadiene/% | Cis-1, 4-butadiene/% | Trans-1, 4-butadiene/% | *T*g/℃ | Predicted *T*g/℃ |
| 1 | 30.6 | 41.3 | 10.2 | 48.6 | -35.9 | -37.05 |
| 2 | 23 | 12.2 | 10.7 | 54.1 | -59.15 | -51.47 |
| 3 | 23.7 | 12.6 | 10.5 | 53.2 | -56.53 | -51.37 |
| 4 | 39.9 | 9.3 | 12.5 | 38.3 | -40.28 | -42.10 |
| 5 | 22.4 | 45.8 | 10.5 | 21.3 | -30.56 | -32.86 |
| 6 | 22.9 | 48.4 | 11.4 | 17.3 | -33.8 | -29.78 |
| 7 | 26.9 | 64.1 | 17.8 | 18 | -22 | -24.30 |
| 8 | 23.5 | 18.7 | 19.4 | 61.8 | -49.8 | -46.77 |
| 9 | 25 | 63 | 15.2 | 21.8 | -4.7 | -23.02 |
| 10 | 25 | 13.5 | 37 | 49.4 | -84.3 | -58.98 |
| 11 | 24.64 | 7.43 | 29.41 | 38.53 | -67.33 | -54.67 |
| 12 | 27.25 | 43.22 | 12.41 | 17.12 | -28.8 | -28.65 |
| 13 | 24.9 | 59 | 19.4 | 21.6 | -26.71 | -26.56 |
| 14 | 35.1 | 50.9 | 22.7 | 26.4 | -22.36 | -23.11 |
| 15 | 25.6 | 36.5 | 23.1 | 14.8 | -26.64 | -28.31 |
| 16 | 22.1 | 61.5 | 21.3 | 17.2 | -28.5 | -29.09 |
| 17 | 20.12 | 62.54 | 13.22 | 24.23 | -29.24 | -30.20 |
| 18 | 21.55 | 63.12 | 11.99 | 24.89 | -28.46 | -29.92 |
| 19 | 21.54 | 62.41 | 12.56 | 25.02 | -28.28 | -30.24 |
| 20 | 20.56 | 62.98 | 12.87 | 24.15 | -31.19 | -29.62 |
| 21 | 21.57 | 63.2 | 11.96 | 24.85 | -30.95 | -29.89 |
| 22 | 27.2 | 68.7 | 6.5 | 31.9 | -20.78 | -15.66 |
| 23 | 36.4 | 24.9 | 38.7 | 36.4 | -31.99 | -33.02 |
| 24 | 25.5 | 39.4 | 12 | 48.6 | -46.94 | -43.18 |



**Figure S1:** Prediction intervals (95% confidence) for the training set samples using the GPR-XGBoost mixed model.



**Figure S2:** Prediction intervals (95% confidence) for the test set samples using the GPR-XGBoost mixed model.