

## Supplementary Materials for:

# Thermal Shock Resistance of Various Two-Dimensional Materials: A Comparative Analysis

Ali Ghavipankeh<sup>1</sup>, Sadegh Sadeghzadeh<sup>2\*</sup>, Nader Malih<sup>3</sup>

1- Research assistant in Nanotechnology Engineering, Smart Micro/Nano Electromechanical Systems (SMNEMS) Laboratory, School of Advanced Technologies, Iran University of Science and Technology, Tehran, Iran

2,\*- Associate Professor of Nanotechnology Engineering, Smart Micro/Nano Electromechanical Systems (SMNEMS) Laboratory, School of Advanced Technologies, Iran University of Science and Technology, Tehran, Iran, Postal Code: 16846-13114.

3- Department of Physics, Faculty of Science, University of Kurdistan, 66177-15175, Sanandaj, Kurdistan, Iran

\* [sadeghzadeh@iust.ac.ir](mailto:sadeghzadeh@iust.ac.ir)

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\*Corresponding author

<sup>1</sup>Email corresponding authors: [Sadeghzadeh@iust.ac.ir](mailto:Sadeghzadeh@iust.ac.ir)

Tel: +982173225812

## Supplementary tables

Table S1. The Tersoff potential parameters[1]

| Parameter                         | Carbon (C)              | Boron (B)             | Nitrogen (N)           |
|-----------------------------------|-------------------------|-----------------------|------------------------|
| A (eV)                            | 1393.6                  | 1393.6                | 1830.8                 |
| B (eV)                            | 346.7                   | 3.467                 | 471.18                 |
| $\lambda_1$ ( $\text{\AA}^{-1}$ ) | 3.4879                  | 2.2119                | 3.2394                 |
| $\lambda_2$ ( $\text{\AA}^{-1}$ ) | 2.2119                  | 1.5                   | 1.3258                 |
| $\lambda_3$ ( $\text{\AA}^{-1}$ ) | 0.0                     | 0.0                   | 0.0                    |
| $\beta$                           | $1.5724 \times 10^{-7}$ | $1.15 \times 10^{-6}$ | $1.178 \times 10^{-7}$ |
| n                                 | 0.72751                 | 0.8                   | 0.83134                |
| c                                 | 38049                   | 33000                 | 130000                 |
| d                                 | 4.3484                  | 3.5                   | 16.217                 |
| h                                 | -0.57058                | -0.3                  | -0.59825               |
| R ( $\text{\AA}$ )                | 1.8                     | 2.0                   | 1.95                   |
| D ( $\text{\AA}$ )                | 0.2                     | 0.2                   | 0.15                   |

Table S2. The Stillinger–Weber (SW) potential parameters for Boron[2]

| Parameter        | Value                      |
|------------------|----------------------------|
| $\epsilon$       | 2.4583                     |
| $\sigma$         | 2.62                       |
| a                | 2.0                        |
| $\lambda$        | 31.5                       |
| $\gamma$         | 1.2                        |
| $\cos(\theta_0)$ | -1/3 ( $\approx -0.3333$ ) |
| A                | 7.049556277                |
| B                | 0.6022245584               |
| p                | 4.0                        |
| q                | 0.0                        |

Table S3. Simulation Cell Size and number of particles

| Structure name or molecular formula | Simulation Boxes Dimension ( $\text{\AA}^3$ ) |                | Particles number |          |
|-------------------------------------|---|----------------|------------------|----------|
|                                     | Zigzag  | Armchair       | Zigzag           | Armchair |
| Borophene(B)                        | 365.4*25.82*110                               | 367.2*28.6*110 | 4095             | 4560     |
| Biphenylene(C)                      | 367.6*27.9*15                                 | 374.7*26.6*15  | 3491             | 3401     |
| BC <sub>3</sub>                     | 363.5*26.7*15                                 | 363.2*25.7*15  | 3407             | 3279     |
| BN                                  | 363.2*25.9*100                                | 366.0*27.4*100 | 3503             | 3739     |
| Graphene(C)                         | 359.2*25.1*20                                 | 369.3*27.4*100 | 3575             | 3783     |
| C <sub>3</sub> N                    | 381.0*25.8*100                                | 377.0*29.8*14  | 3695             | 4223     |
| BC <sub>6</sub> N(a)                | 372.3*26.2*15                                 | 374.2*25.25*15 | 3551             | 3439     |
| BC <sub>6</sub> N(b)                | 370.7*26.15*15                                | 373.2*25.13*15 | 3551             | 3439     |
| BC <sub>6</sub> N(c)                | 372.7*26.2*15                                 | 374.2*25.2*3.1 | 3551             | 3439     |

## Supplementary figures

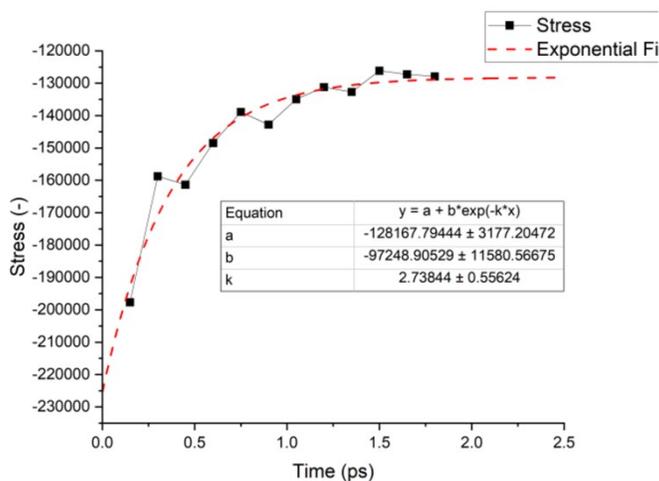
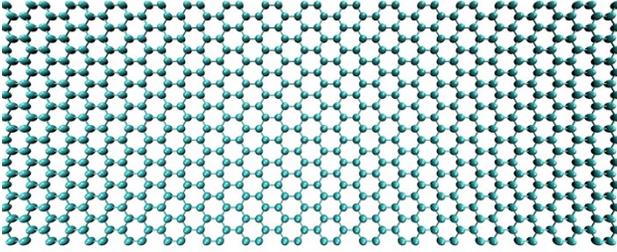
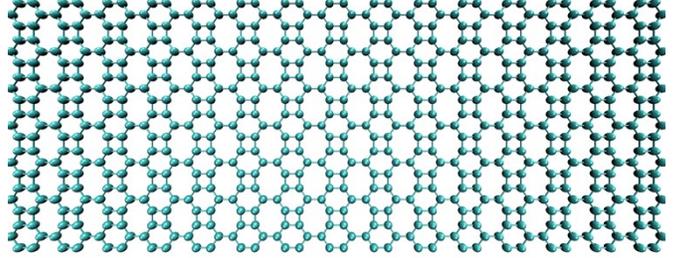


Figure S1. Fitting the stress peaks of zigzag Graphene to equation 1.

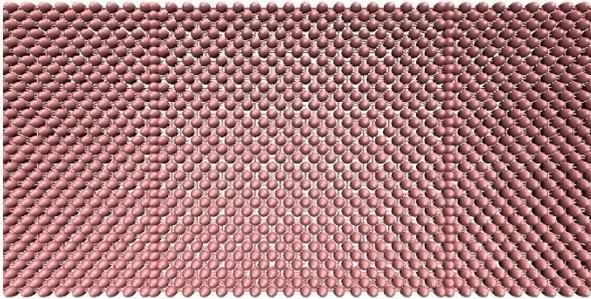
a) graphene



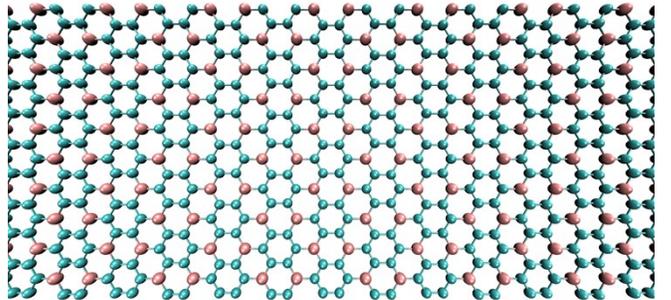
b) Biphenylene



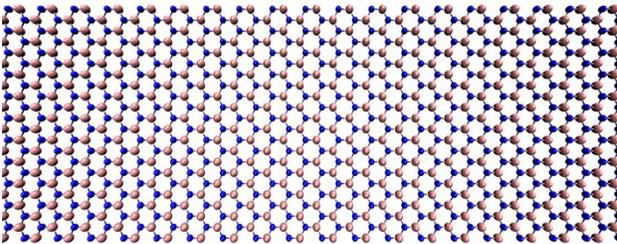
c) Borophene



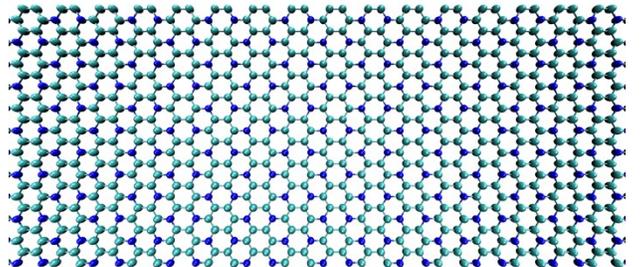
d) BC3



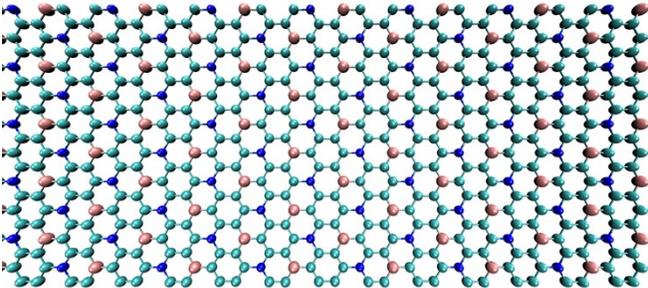
e) h-BN



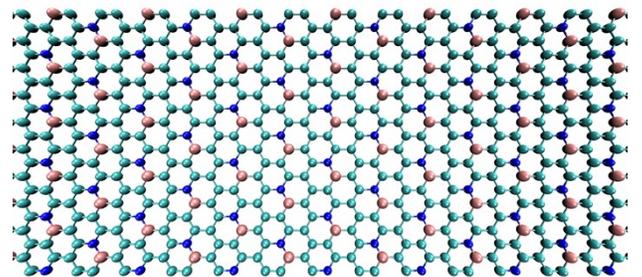
f) C3N



g) BC6N (1)



h) BC6N (2)



h) BC6N (3)

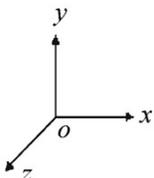
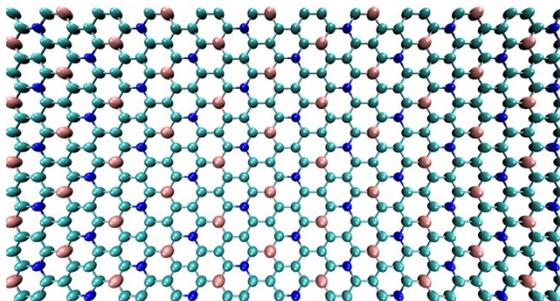


Figure S2. The initial structure of the investigated 2D materials in this work (armchair orientation). a) graphene, b) biphenylene, c) borophene, d) BC<sub>3</sub>, e) h-BN, f) C<sub>3</sub>N, g, h, i) BC<sub>6</sub>N in 3 different structures. (cyan atoms as Carbon, pink as Boron, blue as Nitrogen)

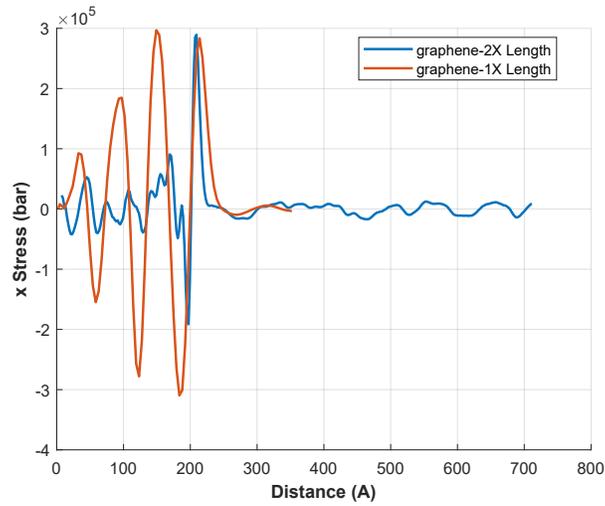


Figure S3. Effect of the Length of the Simulation Cell (in this case, Graphene) on the longitudinal Wave Direction.

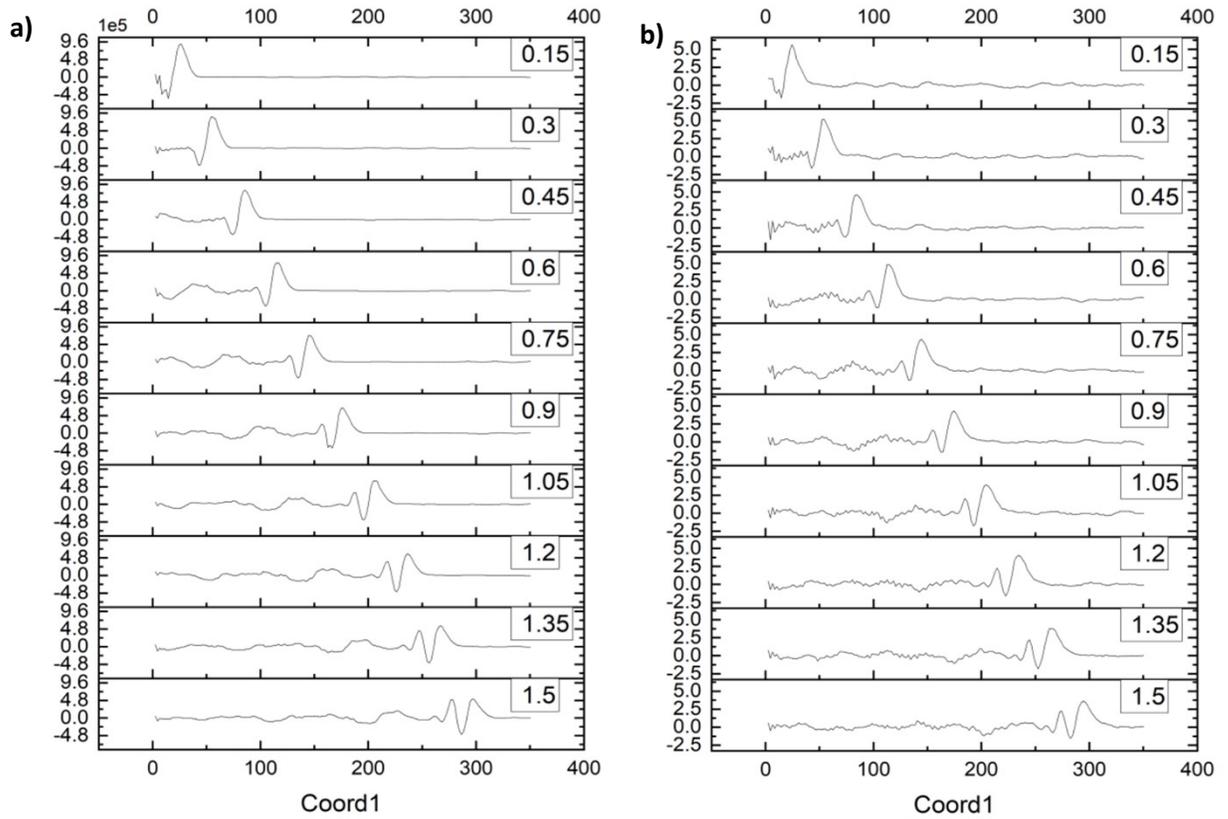


Figure S4. Effect of the two temperatures on the peak wave (in this case, h-BN) regarding the longitudinal wave direction: a) 1000 K and b) 100 K.

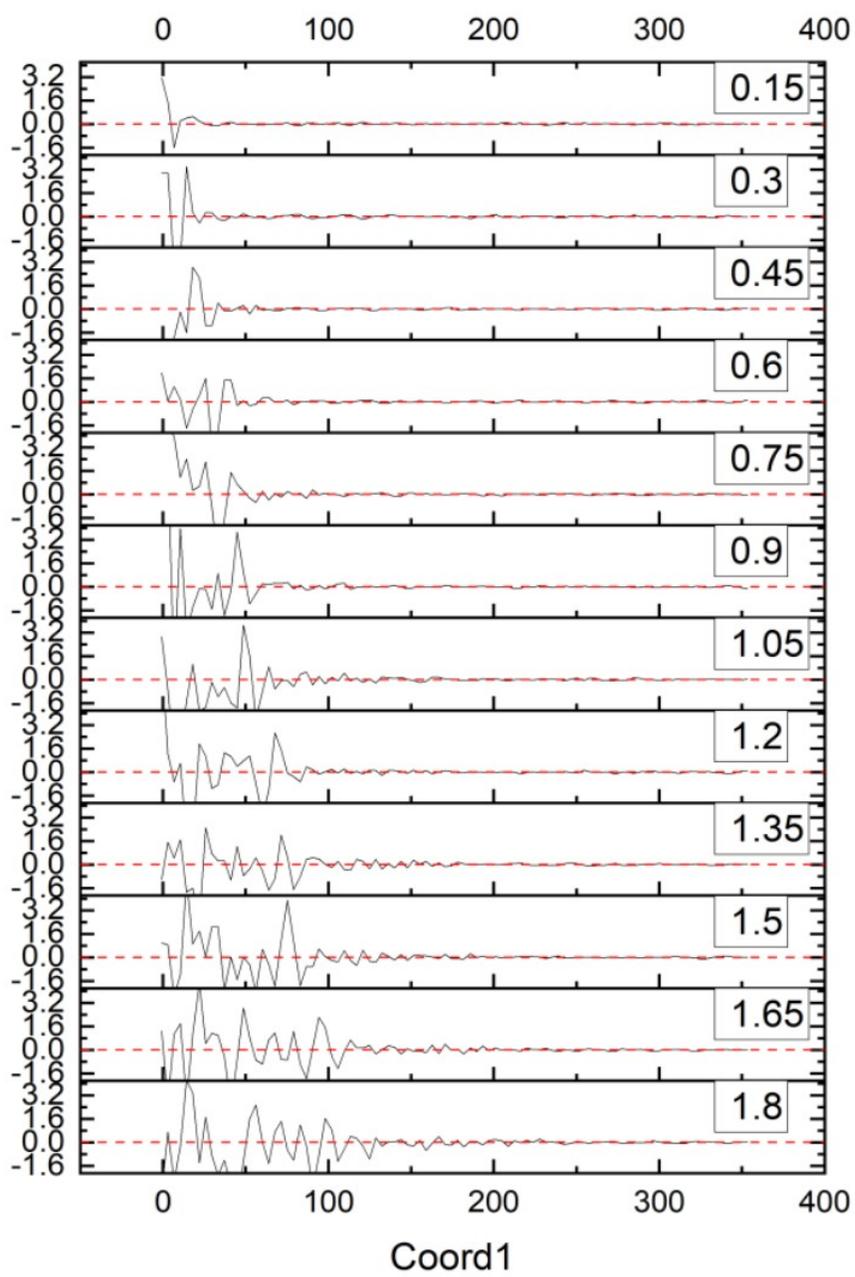


Figure S5. Shear stress ( $xy$ ) in biphenylene over different times.

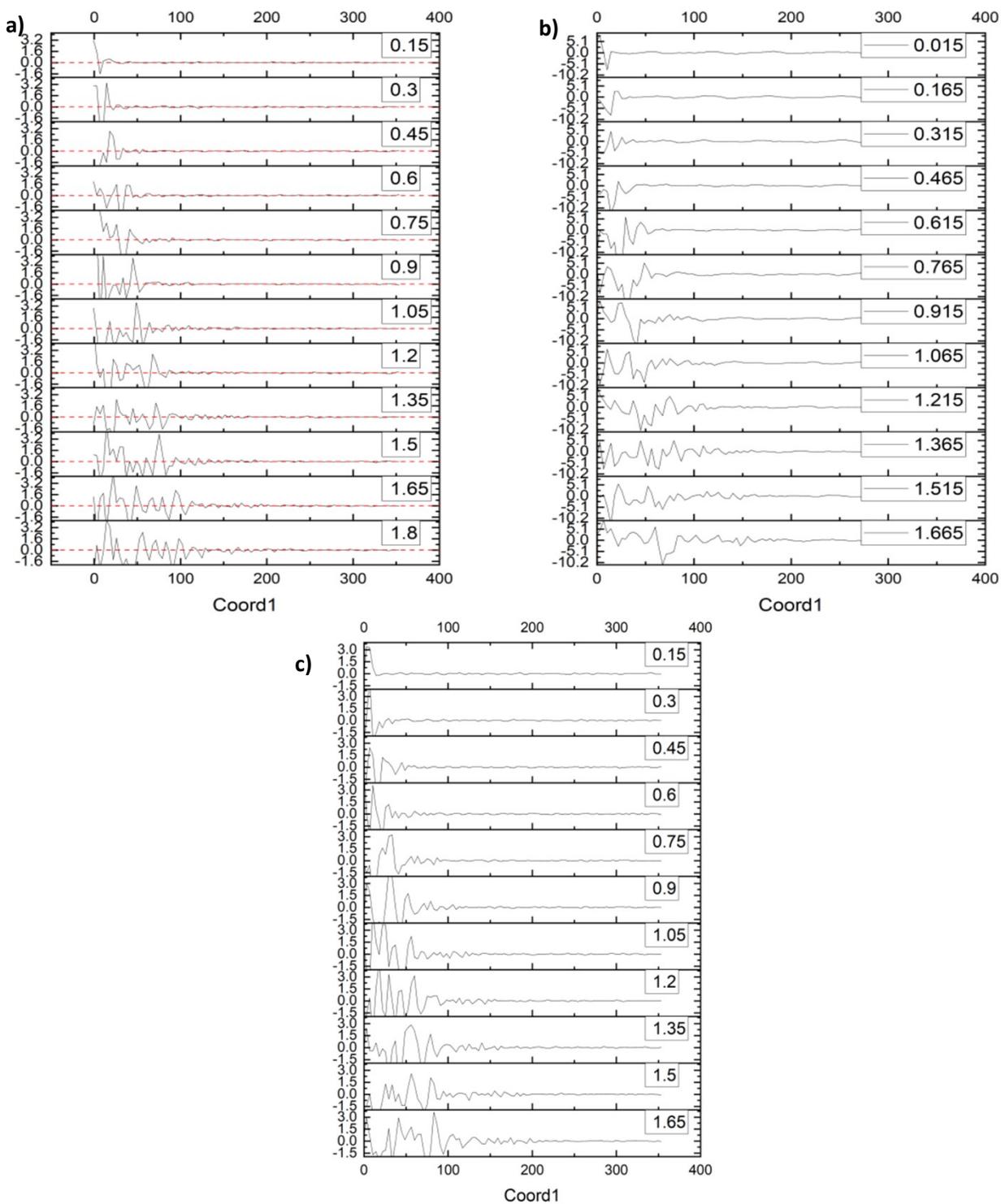


Figure S6. Shear stress wave diagram for the biphenylene structure at different times. A) Prototype with a time step of 0.5 fs, B) A time step of 0.05 fs, which is ten

times smaller than the original sample, and C) A repeated experiment with newly randomized initial velocities.

## Supplementary movie

Movie S1 includes longitudinal and shear stress colour plots and stress coordination plot animations for both armchair and zigzag directions, as well as an atomic displacement plot for the investigated materials.

## References

1. Kinaci, A., et al., *Thermal conductivity of BN-C nanostructures*. Physical Review B—Condensed Matter and Materials Physics, 2012. **86**(11): p. 115410.
2. Moon, W.H. and H.J. Hwang, *A modified Stillinger–Weber empirical potential for boron nitride*. Applied surface science, 2005. **239**(3-4): p. 376–380.