

## Supporting Information

### Determining the structure of functionalized graphene for tailored thermomechanical properties using ML techniques

*Ravil Ashirmametov*<sup>a\*</sup>, *Alexandr Alpatov*<sup>b</sup>, *Farrokh Yousefi*<sup>a</sup>, *Narges Vafa*<sup>a</sup>, *Siamac Fazli*<sup>b</sup>, *Konstantinos Kostas*<sup>a</sup>

<sup>a</sup>Department of Mechanical and Aerospace Engineering, School of Engineering and Digital Sciences, Nazarbayev University, Astana, Kazakhstan.

<sup>b</sup>Department of Computer Science, School of Engineering and Digital Sciences, Nazarbayev University, Astana, Kazakhstan.

\*Corresponding author. E-mail: ravil.ashirmametov@nu.edu.kz

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## 1 Models' Hyperparameters

### 1.1 Hydrogen Functionalization - Label Encoding

- **Target Property: Young's Modulus**

- Model: SVM
- Kernel: Linear
- Box constraint: 287.3936
- Epsilon: 0.066865
- Standardization: True

- **Target Property: Maximum Stress**

- Model: SVM
- Kernel: Gaussian
- Kernel Scale: 54.6894
- Box constraint: 41.1479
- Epsilon: 0.050525
- Standardization: False

- **Target Property: Strain at Maximum Stress**

- Model: SVM
- Kernel: Quadratic
- Kernel Scale: 103.0347
- Box constraint: 0.0137
- Epsilon: 0.0014
- Standardization: True

- **Target Property: Kappa**

- Model: SVM
- Kernel: Gaussian
- Kernel Scale: 80.4264
- Box constraint: 566.4505
- Epsilon: 0.091427
- Standardization: True

## 1.2 Hydrogen Functionalization - Bag-of-Words Encoding

- **Target Property: Young's Modulus**
  - Model: Ridge
  - Alpha: 1.0
  - PolynomialFeatures degree: 2
- **Target Property: Maximum Stress**
  - Model: kNN
  - k: 9
  - PolynomialFeatures degree: 1
- **Target Property: Strain at Maximum Stress**
  - Model: kNN
  - k: 11
  - PolynomialFeatures degree: 1
- **Target Property: Kappa**
  - Model: Ridge
  - Alpha: 0.1
  - PolynomialFeatures degree: 3

## 1.3 Methyl Functionalization - Label Encoding

- **Target Property: Young's Modulus**
  - Model: SVM
  - Kernel: Linear
  - Box constraint: 3.6977
  - Epsilon: 0.055999
  - Standardization: True
- **Target Property: Maximum Stress**
  - Model: SVM
  - Kernel: Linear
  - Box constraint: 107.0537
  - Epsilon: 0.0064465
  - Standardization: True
- **Target Property: Strain at Maximum Stress**
  - Model: SVM
  - Kernel: Gaussian
  - Kernel Scale: 92.0
  - Standardization: True
- **Target Property: Kappa**
  - Model: SVM
  - Kernel: Linear
  - Box constraint: 6.6544
  - Epsilon: 0.015733
  - Standardization: True

## 1.4 Methyl Functionalization - Bag-of-Words Encoding

- **Target Property: Young's Modulus**
  - Model: Ridge
  - Alpha: 0.1
  - PolynomialFeatures degree: 3
- **Target Property: Maximum Stress**
  - Model: SVR
  - Kernel: Linear
  - C: 1
  - Epsilon: 0.1
  - PolynomialFeatures degree: 2
- **Target Property: Strain at Maximum Stress**
  - Model: Ridge
  - Alpha: 10
  - PolynomialFeatures degree: 3
- **Target Property: Kappa**
  - Model: SVR
  - Kernel: RBF (Radial Basis Function)
  - C: 10
  - Epsilon: 1
  - PolynomialFeatures degree: 1