Machine Learning Predicted Inelasticity in Defective Two-Dimensional Transition Metal Dichalcogenides using SHAP Analysis

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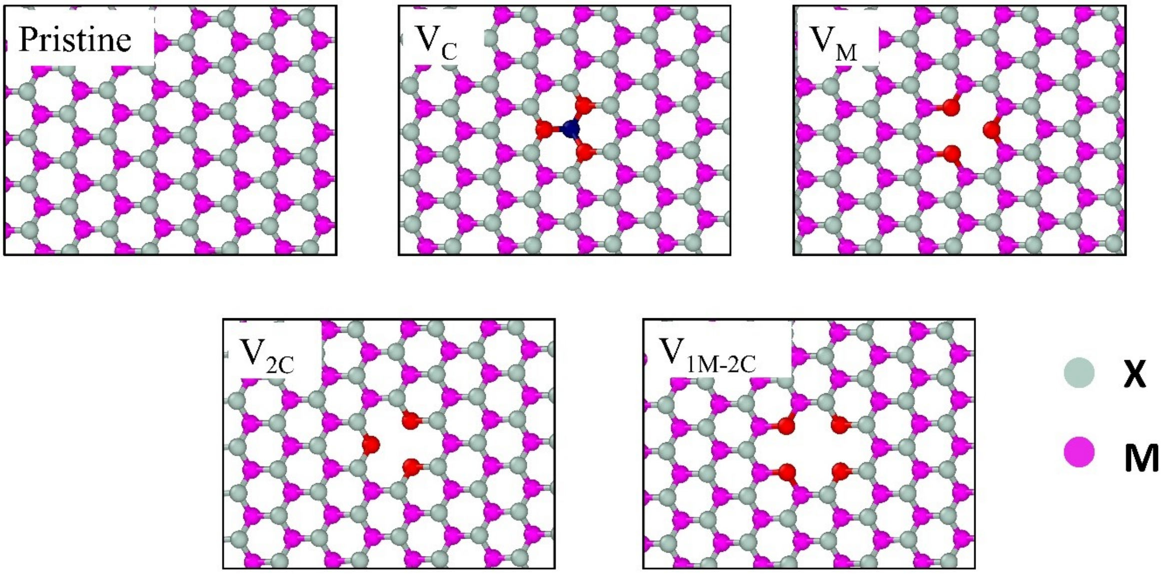

Figure S1 Schematic representations of pristine and defective samples of H-MX_2. Here, grey-colored spheres indicate chalcogen atoms (i.e., X=O, S, Se, and Te), purple sphere indicates metal atoms (i.e., M = Sc, Ni, V, and Cr), and red atoms indicate the unbonded atoms.

Feed Forward Neural Network (FFNN) Modelling Details:

Even though we focused mainly on DenseNet & XGBoost, we also made a model on Feed Forward Neural Network to get an idea of how our model works in secluded points without any ensemble or hidden layer temporal connections, and solely based on the material properties & strain values. Then, we use an activation function to **'activate'** the neuron, simply to introduce non-linearity to the neuron function. These 'linear' & 'non-linear' parts construct a neuron that processes the information, and with backpropagation & optimization of weights, it learns to get an output close to the target sample space. The mathematical representation is as follows: the individual feature inputs $X_1, X_2, X_3, \dots X_n$ are each multiplied by corresponding weights $W_1, W_2, W_3, \dots W_n$, and the results are combined as the dot product of vectors W and $\boldsymbol{X}$. Here, $\boldsymbol{X} = [X_1, X_2, X_3, \dots X_n]^T$ represents the input vector, and $\boldsymbol{W} = [W_1, W_2, W_3, \dots W_n]$ symbolizes the weight vector. The outcome of this dot product is then added to a threshold bias b (to make it more generalized) and used as an input to the activation function: $Y = A\,(\boldsymbol{W}.\,\boldsymbol{X} + \boldsymbol{b})$, where A represents the activation function, and $\boldsymbol{Y}$ is the resulting output. Moving on, a feedforward neural network (FFNN) is a multilayer artificial neural network where information flows unidirectionally, from inputs to outputs, without any feedback loops. In this network architecture, neurons within the same layer are not interconnected but are connected to all neurons in the adjacent layers.

Dataset Preparation for FFNN Model: The initial step in developing an Artificial Neural Network (ANN) model is to create a dataset. Data from the tensile test simulations of monolayer TMDs (Transition Metal Dichalcogenides) was used in this context. The dataset comprises ten distinct TMDs, each tested in various chiral directions, three different strain rates, and four types of defects, including pristine structures. Only specific strain values with uniform step sizes were selected across all simulated data files for consistency.

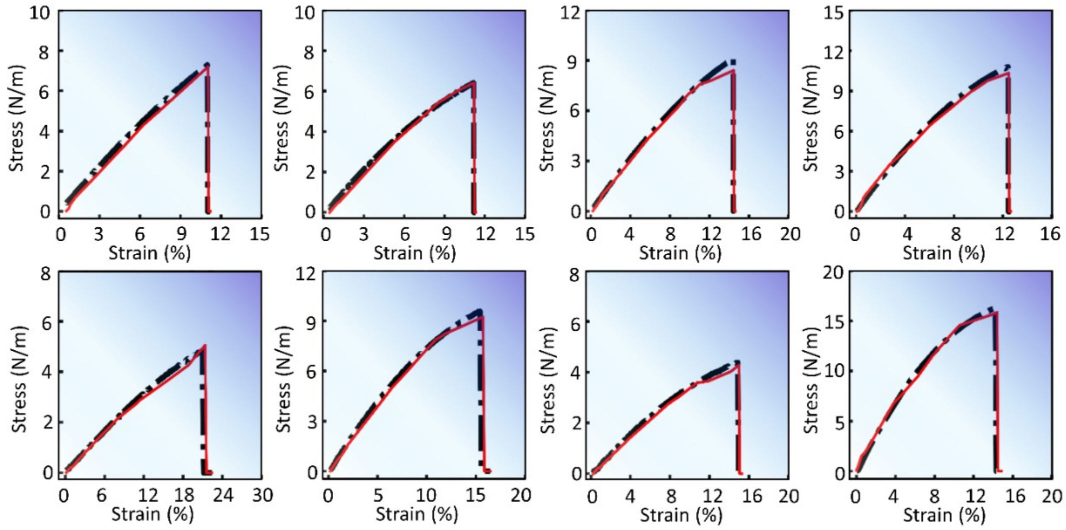

Figure S2. *DenseNet* model predictions to capture the variation in the strain rate with chiral directions for pristine samples only. Subfigures (a-d) and (e-h) represent the response of 2D TMDCs along *ac* and *zg,* respectively, for strain rates increase from the left to right in the range of $10^7 s^{-1}$ to 10^{10} s^{-1}. Materials from a to h are: H-$NbSe_2$, H-NiS_2, H-VS_2, H-VO_2, H-$ScTe_2$, H-CrS_2, H-$NiSe_2$, H-CrO_2 respectively

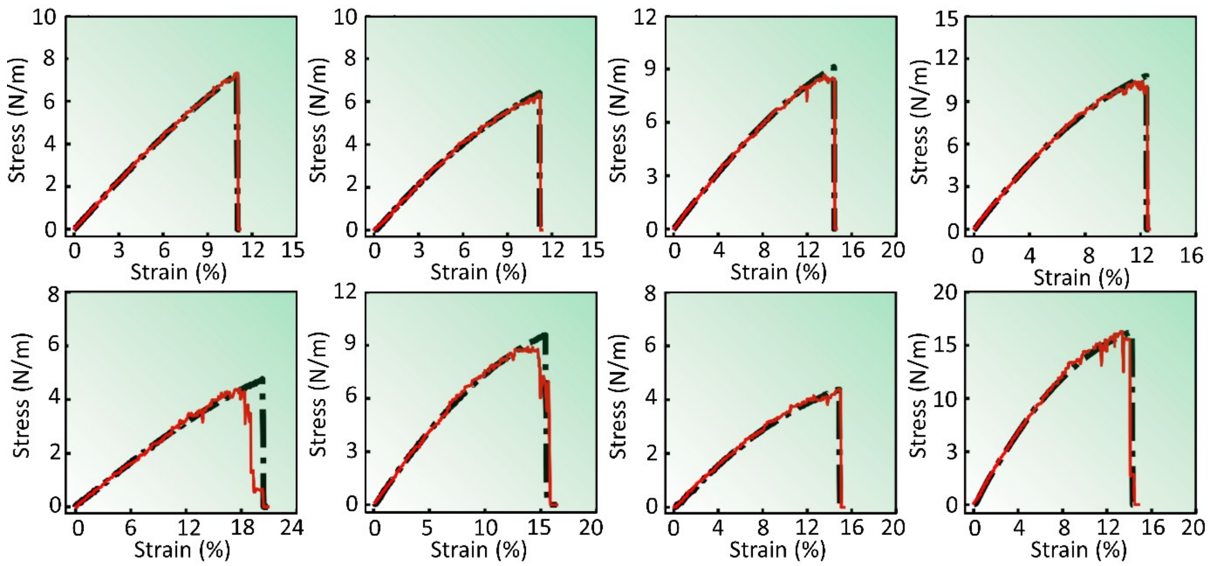

Figure S3. XGBoost model predictions capture the variation in the strain rate with chiral directions for pristine samples only. Subfigures (a-d) and (e-h) represent the response of 2D TMDCs along *ac* and *zg,* respectively, for strain rates increase from the left to right in the range of 10^7 s^{-1} to 10^{10} s^{-1}. Materials from a to h are: H-$NbSe_2$, H-NiS_2, H-VS_2, H-VO_2, H-$ScTe_2$, H-CrS_2, H-$NiSe_2$, H-CrO_2 respectively.

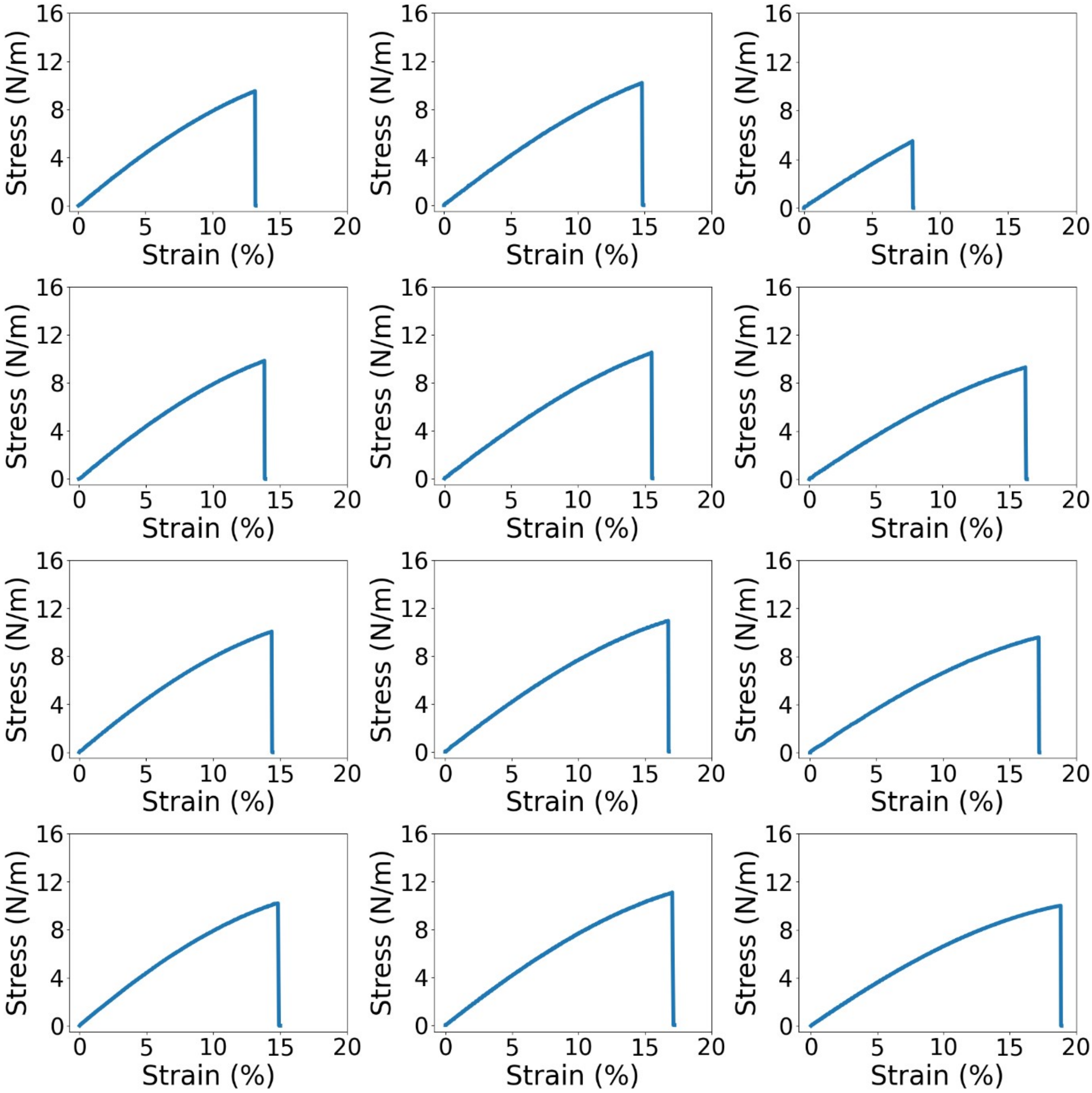

Figure S4: The actual stress-strain plots of pristine CrS_2, $CrSe_2$, and $CrTe_2$ (from left to right) for different strain rates 10^7 s^{-1} to 10^{10} s^{-1}. (from top to bottom). All the subfigures represent stress-strain response in the armchair direction.

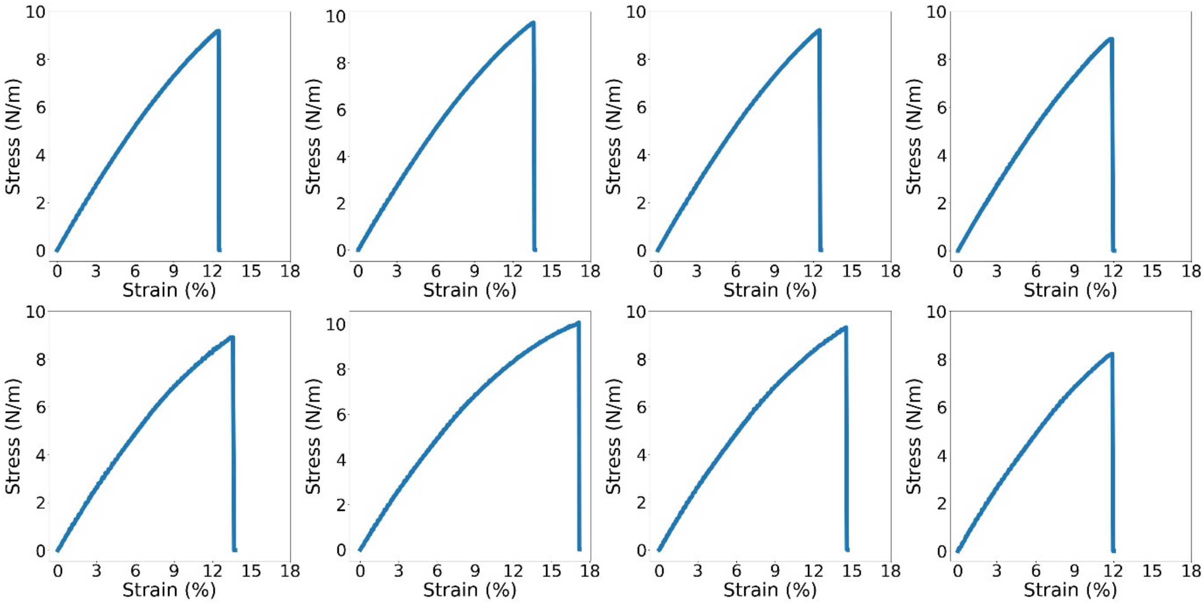

Figure S5: The actual stress-strain plots for different defects V_M, V_C, V_{2C} and V_{1M-2C} (left to right) and chiral orientation armchair and zigzag (top to bottom). The 2D TMDC material and strain rate are fixed as CrS_2 and 10^{10}/s, respectively.