# Applying machine learning techniques to predict the properties of energetic materials

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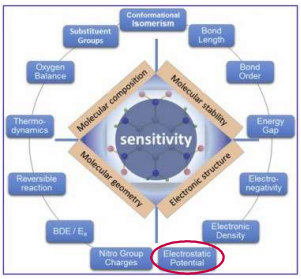
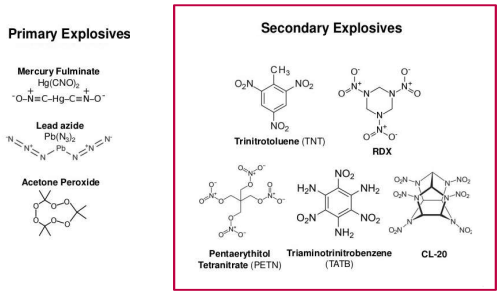
## 1.Abstract

The development of new energetic materials (EMs) is accompanied by significant hazards, prompting interest in their computational design. Before reliable in silico design strategies can be realized, however, approaches to understand and predict EM response to mechanical impact must be developed. We present here a proof of concept that machine learning techniques can be used to predict the properties of CNOHF energetic molecules from their molecular structures. We focus on a small but diverse dataset consisting of 218 molecular structures spread across ten compound classes. This work describes the development of models for prediction of impact sensitivity using approximations of the electrostatic potentials.



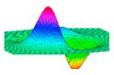

## 2.Types of Explosives




## 3. A Methodological Approach to Developing Model using in this study

- Molecular Structures

- Geometry Optimization



- Molecular Description Generation :
  Descriptors of the electrostatic potential : $V_S^+$, $V_S^-$, $V_S$, $A_s^+$,$A_s^-$
  Frontier Molecular Orbitals : HOMO, LUMO
  Fukui indices descriptors $f^+$,$f^-$,$f^0$, $q(C)_{max}$
- Molecular Description Selection
  Descriptors of the electrostatic potential : $V_S^+$, $V_S^-$, $V_S$
- Model Development

$$h_{50\%} = a_1 + a_2 \exp(-a_3(|V_s^+| - |V_s^-|))$$

- Model Validation

## 4.Calculations

The molecular structures of the compounds used in this study were obtained from the Huang & Massa data[2] and from the Mathieu dataset[3]. Optimized molecular geometries and electrostatic potentials were computed at the density functional B3LYP/6-31G* Level.

## 5.Electrostatic potential

The electrostatic potential, V(r), is defined as[3] : $V(\mathbf{r}) = \sum_i \frac{Z_i}{|\mathbf{R}_i - \mathbf{r}|} - \int \frac{\rho(\mathbf{r}')\,d\mathbf{r}'}{|\mathbf{r}' - \mathbf{r}|}$

Where $Z_i$ and $R_i$ denote the charge and position of the nucleus of atom i and ρ(r) represents the electronic density.

The electrostatic potential is calculated using quantum mechanical theory and is used to analyze the electron density distribution in a molecule.

## 6.Results

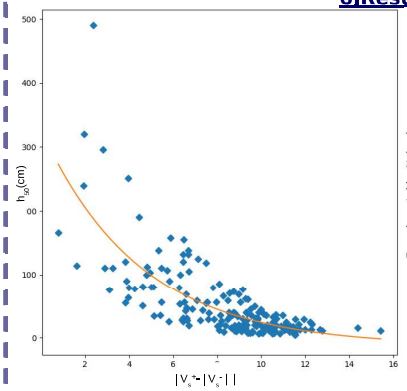



Fig 1 : Measured $h_{50\%}$ results vs $|V_s^+|-|V_s^-|$. Predictions using the model (1) is shown as the solid line :

$$h_{50\%} = a_1 + a_2 \exp(-a_3(|V_s^+| - |V_s^-|)) \quad (1)$$

where best fit parameters are $a_1$= 12.81cm, $a_2$ = 339.93cm and $a_3$ =0.22 (kcal/mol)

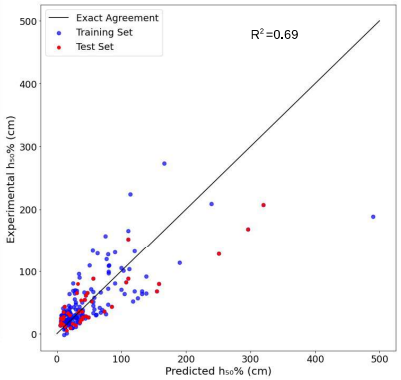



Fig 2 : Comparaison of calculated $h_{50\%}$ vs. experimental $h_{50\%}$ derived from the model (1). The correlation coefficient ($R^2$) for this fit is 0.69.

## 7.Conclusion

In summary, we describe the development of a Nonlinear regression/DFT model for the prediction of impact sensitivity using approximation of electrostatic potentials. The Nonlinear regression section consists of training a model (1) on a database of experimental data ($h_{50\%}$), developed in ref 1,2. The trained model ($N_{train}$ = 185, $N_{test}$ = 33) results in a good correlation, $R^2$ = 0.69.

## 8. Perspectives

Predicting the impact sensitivities of energetic materials using the machine learning techniques through :
- Frontier Molecular Orbitals (HOMO, LUMO and their energy gap)
- Fukui indices descriptors
- Activation energy of thermal decomposition

## References :

1) Huang, L. & Massa, L. Int. J. Ener. Mat. Chem. Prop. 12, 197–262 (2013)
2) Mathieu, D. Ind. & Eng. Chem. Res. 56, 8191–8201 (2017).
3) Rice, B. M., & Hare, J. J. (2002).. The Journal of Physical Chemistry A, 106(9), 1770-1783.
4) Elton, D. C., Boukouvalas, Z., Butrico, M. S., Fuge, M. D., & Chung, P. W. (2018). Scientific reports, 8(1), 1-12.