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AI-driven design and optimization of flame retardant epoxy nanocomposites and textiles

A. Bifulco,[1,*] C. Imparato,[2] I. Climaco,[1] A. Casciello,[1] V. Nebbioso,[1] J. Passaro,[2] P. Russo,[2] S. Gaan,[3] G. Malucelli,[4] A. Aronne[1]

[1] *Department of Chemical, Materials and Production Engineering (DICMaPI), University of Naples Federico II, P.le Tecchio 80, 80125 Naples, Italy*
[2] *Institute of Polymers, Composites and Biomaterials (IPCB), National Research Council (CNR), Via Campi Flegrei 34, 80078, Pozzuoli, Naples, Italy*
[3] *Laboratory for Advanced Fibers, Empa Swiss Federal Laboratories for Materials Science and Technology, Lerchenfeldstrasse 5, 9014 St. Gallen, Switzerland*
[4] *Department of Applied Science and Technology, Politecnico di Torino, Viale Teresa Michel 5, 15121 Alessandria, Italy*
**aurelio.bifulco@unina.*

The development and optimization of flame retardant (FR) materials usually require time-consuming, expensive, and destructive measurements. However, in most cases the material available for flammability and fire performance testing is limited. In this view, machine learning (ML) tools can be very useful to predict the fire parameters of polymeric materials or textiles, starting from an input dataset of properties (e.g., thermal or physico-chemical characteristics accessible in the literature) belonging to similar systems. Herein, we demonstrate the suitability of ML algorithms for the design and development of FR hybrid epoxy nanocomposites and functional textiles. Artificial neural network-based systems built on fully connected feed-forward artificial neural networks can successfully be employed for the prediction of heat release capacity of FR hybrid $Mg(OH)_2$-epoxy nanocomposites. Electrospun fibres can be used to coat hemp blankets and obtain a fire shielding multilayer material. Despite the incomplete starting datasets, ML with generative AI (ChatGPT) approaches allow to exploit made-on-purpose decision trees and artificial neural networks to finely predict the time to ignition and the peak of heat release rate of the multilayer material.

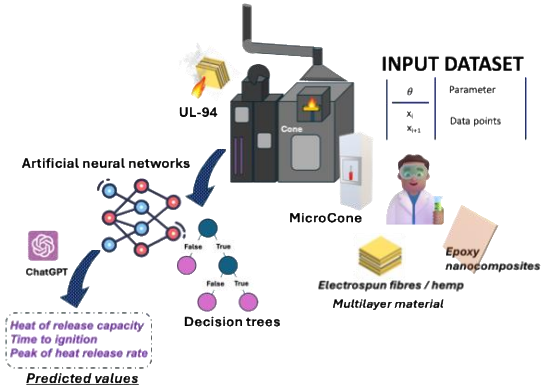

Figure 1. Decision trees and artificial neural networks as predictive methods in flame retardancy.

References

[1] A. Bifulco, A. Casciello, C. Imparato, S. Forte, S. Gaan, A. Aronne, G. Malucelli *Polymer Testing* **2023**, *127*, 108175.
[2] A. Bifulco, I. Climaco, A. Casciello, J. Passaro, D. Battegazzore, V. Nebbioso, P. Russo, C. Imparato, A. Aronne, G. Malucelli *Journal of Materials Science* **2025**, *60*, 1019–1040.