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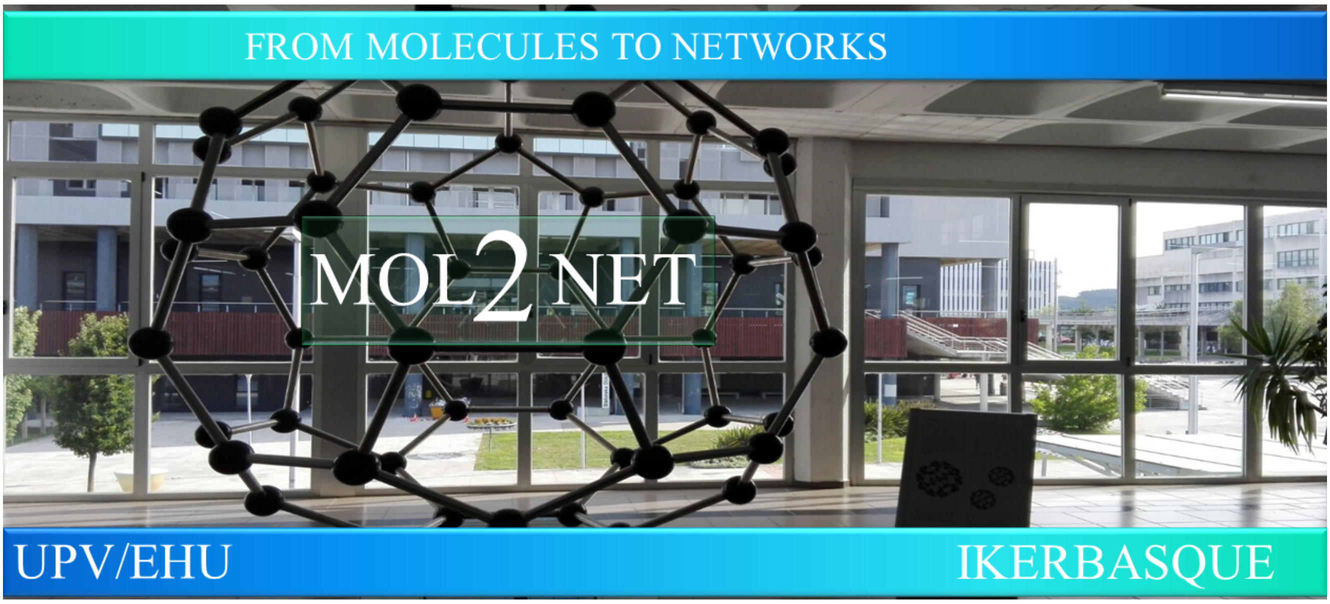

Multidisciplinary Exploration of Entropy: From Carbon Nanotubes to High Entropy Catalysts

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Abstract.

The discussion between the three scientific articles reveals the innovative use of entropy in different scientific contexts and applications. In the article by González-Durruthy et al. (2017), Shannon entropy is used to transform the Raman spectra of carbon nanotubes, developing nano-PT-QSPR regression models that successfully predict the effect of nanotubes on mitochondrial respiration. This in silico approach provides a deep understanding of how nanomaterials affect biological systems. On the other hand, Prado-Prado et al. (2011) use the entropy of drug and protein graphs to develop an mt-QSAR model, focused on predicting the FDA drug-target network. This research combines theoretical and experimental studies, demonstrating the usefulness of entropy in predicting drug-target interactions and in understanding the structure of drug target proteins. The article by Roy et al. (2022) highlights the use of entropy in the context of high-entropy alloy-based catalysts for the selective reduction of CO2 to methanol. Machine-assisted machine learning is used to explore the diversity of metal combinations in high-entropy alloys, demonstrating the ability to

predict adsorption energy and identify promising catalysts for methanol synthesis. In comparison, all three studies employ entropy creatively to model and predict phenomena in biological systems, drug-target networks, and high-entropy catalysts. Although each article focuses on a different field, they share the common strength of using entropy as a valuable tool to quantify diversity, complexity, and information in diverse systems, demonstrating its versatility and applicability in scientific research. Furthermore, they highlight the importance of machine learning and in silico approaches to advance the understanding and application of entropy in various scientific fields.

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