



Showcasing research from Professor Yamil J. Colón's laboratory, College of Engineering, University of Notre Dame, Notre Dame, IN, United States.

Open-source generation of sigma profiles: impact of quantum chemistry and solvation treatment on machine learning performance

The first end-to-end open-source Sigma Profile (SP) generator - OpenSPGen was developed. The tool was deployed on a diverse sample of molecules to optimize SP generation settings to enhance machine learning performance for thermophysical property prediction. Higher levels of theory did not translate to improved machine learning performance, and conventional post-processing procedures were found to be best avoided in machine learning applications.

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As featured in:



See Yamil J. Colón *et al.*, *Digital Discovery*, 2025, **4**, 2711.