Combined Machine Learning and Computational Analysis of the Copper (I) Complexes with Optical Properties

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Various coordination complexes have been the subject of experimental and theoretical studies in recent decades because of their fascinating photophysical properties. In this work, a combined machine learning and computational density functional theory approach was applied to investigate the optical properties of Cu(I) complexes. An interpretative machine learning-based quantitative structure–property relationship (ML/QSPR) model was successfully developed that could reliably predict the absorption properties of the Cu(I) complexes and provide a foundation for the theoretical evaluation of the optical properties of Cu(I) complexes. A hypothesis was proposed to explain the differences in the absorption wavelengths between structurally different individual Cu(I) complexes. The efficacy of the developed model was demonstrated by high R^2 and Q^2 values for the training and test sets. Moreover, the developed model was applied to a large virtual library to search for better analogs with desired optical properties. This combined machine learning and computational approach shows great potential for the rational design of new Cu(I) complexes with the desired optical properties. Moreover, the developed methodology could be extended to other transition-metal complexes.