

Graph convolution networks for property estimation : improved property estimation and uncertainty analysis

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Pure property estimation is essential in chemical process when experimental approach is difficult. Group contribution methods have been held well so far. As computer technology develops over time, more accurate prediction has been possible by using artificial neural networks architecture. However, due to shortage of experimental data, only few papers have been reported the successful predictions of thermodynamic properties with artificial neural networks. In this work, we represent a new method with hybrid stance of group contribution method and molecular graph neural networks for estimation of pure thermodynamic properties: normal boiling point, normal melting point, critical temperature, critical pressure, critical volume, closed-cup flash point, standard enthalpy of fusion, standard enthalpy of formation, standard Gibbs energy of formation. The application of graph convolution networks successfully overcome the isomer discrimination problem, while the concept of group contribution effectively reduced the number of parameters. Moreover, to ensure reliability, uncertainty analysis is held.