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A Quantitative Structure-Adsorption Study on Novel and Emerging Adsorbent Materials

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Abstract : Considering a large amount of adsorption data of adsorbate gases on adsorbent materials in literature, it is interesting to predict such adsorption data without experimentation. A quantitative structure-activity relationship (QSAR) is developed to correlate molecular characteristics of gases and existing knowledge of materials with their respective adsorption properties. The application of Random Forest, a machine learning method, on a set of adsorption isotherms at a wide range of partial pressures and concentrations is studied. The predicted adsorption isotherms are fitted to several adsorption equations to estimate the adsorption properties. To impute the adsorption properties of desired gases on desired materials, leave-one-out cross-validation is employed. Extensive experimental results for a range of settings are reported.

Keywords : adsorption, predictive modeling, QSAR, random forest
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