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Machine learning-aided modeling of the hydrogen storage in zeolite-based porous media

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Highlights

- Effect of surface and pore properties of zeolites on hydrogen storage is compared.
- BET surface area of zeolites is more vital than pore volume for the H_2 storage.
- Machine learning models are applied to simulate H_2 loading capacity of zeolites.
- H_2 storage increases by increasing zeolites' BET surface area and total pore volume.
- The proposed model predictions are interpretable by the Chahine's rule.

Abstract

Zeolites are among the most popular porous solids for hydrogen storage. Hydrogen attaches to the surface and microporous structure of zeolites. The literature mainly inspected the hydrogen adsorption capacity of zeolites (HACZ) experimentally and paid little attention to its modeling. Furthermore, there is no tool to compare/reveal the role of surface and pore characteristics of zeolites in hydrogen storage. This work applies several well-established artificial intelligence techniques to correlate the HACZ to surface and pore characteristics of zeolites, pressure, and temperature. The topology-tuned multi-layer perceptron neural network is the best model to simulate the hydrogen storage of fourteen systems (NH_4Y, X, and ZSM-5). This model predicts the HACZ of a vast experimental databank with a regression coefficient of 0.99875 and an absolute average relative deviation of 6.43%. Results approve that the role of the BET surface area of zeolites on the HACZ is more vital than the pore volume.