Evaluating Performance Limits of Methane Storage/Separations of Porous Materials Using Artificial Neural Network

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In this work, we show that artificial neural network (ANN) can be used to evaluate the performance limits for methane storage/separations in nanoporous materials. Our newly developed ANN can successfully generate energy "shapes" that can mimic methane potential energy grids of realistic porous materials. In a case study, we chose pure-silica zeolites system due to their completeness of filling the mathematical possible spaces of all materials within that class. The methane adsorption data generated from our ANN matches well with the distributions of real zeolites. This new methodology/framework can be used to estimate the performance limits of materials and will make an important contribution of answering the question of whether or not it would be worthwhile to fund a specific research from the perspective of government/businesses.