Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Prediction of Zeolite Framework Types by a Machine Learning Approach[1] SHUJIANG YANG, MOHAMMED LACH-HAB, IOSIF VAISMAN, ESTELA BLAISTEN-BAROJAS, Computational Materials Science Center, George Mason University, Fairfax, VA 22030 — Zeolites are microporous crystalline materials with highly regular framework structures consisting of molecular-sized pores and channels. Characteristic framework types of zeolites are traditionally determined by the combined information of coordination sequences and vertex symbols. Here we present a machine learning model for classifying zeolite crystals according to their framework types. An eighteen-dimensional feature vector is defined including topological descriptors and physical/chemical properties of zeolite crystals [Microporous and Mesoporous Materials 117, 339 (2009)]. Trained with crystallographic data of known zeolites, the new model can predict the framework types of unknown zeolite crystals with up to 98 % accuracy. Compared with conventional methods, the machine learning model is more robust handling crystal disorder and/or crystal defects in a more effective manner. This model can be adapted for classifying and clustering other crystalline species.

[1]Supported by NSF grant CHE-0626111

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Date submitted: 11 Dec 2008 Electronic form version 1.4