Public Abstract

First Name:Jiasen

Middle Name:

Last Name:Guo

Adviser's First Name:Karl

Adviser's Last Name:Hammond

Co-Adviser's First Name:

Co-Adviser's Last Name:

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Department:Chemical Engineering

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Title:COMPUTATIONAL STUDY OF INFRARED SPECTRA OF SILICA POLYMORPHS VIA CLASSICAL MECHANICS

Zeolites have been widely used as catalysts in the petrochemical industry and adsorbents in environmental protection area. A potential energy model that correctly reflects zeolite framework interactions is the premise for computational studies of the physical and chemical processes occurring inside zeolites. In this work, two published potentials are evaluated in terms of their abilities in predicting infrared spectra and equilibrium geometries of five silica polymorphs. The evaluation of the two potentials and further parametrization and extension result in a new potential which reproduces silica polymorphs' infrared spectra more accurately. This means that the newly-developed potential is a better candidate for the computational modeling of the underlying physics of zeolite applications, which in turn, will help improve the performance of zeolites in various areas.