

Mechanical Properties of Zeolites Investigated by Field Theory and Classical MD Simulation

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Field theory and classical MD simulation considering three-body potential are employed to characterize the response of zeolites under simple tension loading. The ultimate tensile strength (UTS) and elastic modulus are obtained by investigating the stress-strain relation. Elastic response and the failure process are obtained through atomic-level MD simulation. Mechanical behaviors of zeolites under the influence of the temperature and pressure with different specimen size are predicted. There is a good agreement in the results from the field theory and classical MD simulation, while field theory is proved to be much more efficient.

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