COMPUTATIONAL CHEMISTRY

EXPLORATORY PROJECT REPORT DOCUMENTATION.

Molecular simulation of adsorption of methane on zeolite.

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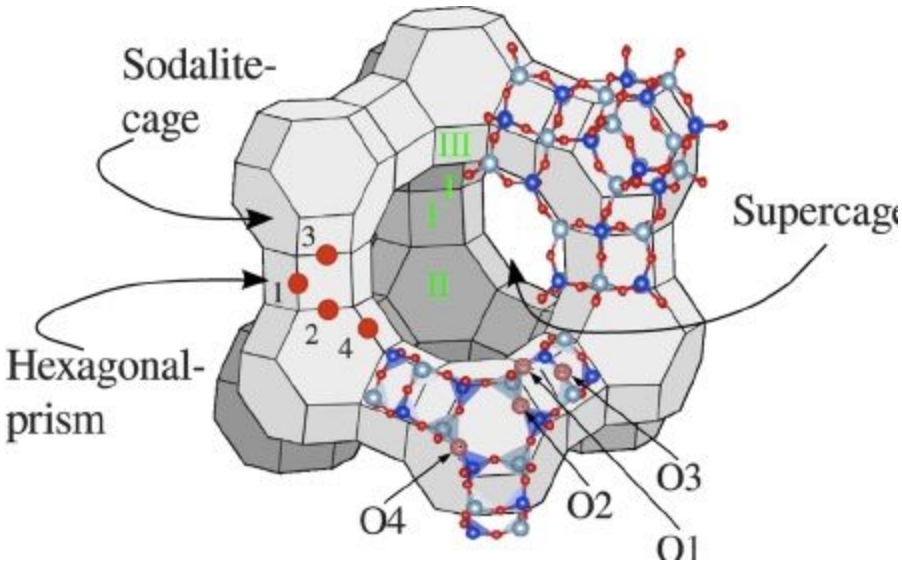


ZEOLITE USED

Sodium Faujasite , O384 Al32 Si160. Na

SOFTWARE USED TO IMPLEMENT THIS

MAPS (MATERIALS AND PROCESS SIMULATION) BY

SCIENOMICS.

IMPORTANCE OF THIS PROJECT -

IN ALUMINOSILICATE FAUJASITE TYPE ZEOLITE, A DETAILED KNOWLEDGE OF THE ADSORPTION MECHANISM OF HYDROCARBONS IS OF GREAT INTEREST IN THE CONTEXT OF PETROCHEMICAL APPLICATION SUCH AS SEPARATION PROCESSES. A PROMINENT APPLICATION IS THE SEPARATION OF BRANCHED ALKANES FROM n-ALKANES, AIMED AT PRODUCING FUELS OF HIGH OCTANE NUMBER.

MCCCS TOWHEE

Maps has an interface with the mcccs-towhee (monte carlo for chemical systems), which carries our computation in different ensemble. After generating the models, the stimulation on towhee was initiated on maps platform itself and the forcefield and towhee input files were generated.

DREIDING FORCE FIELDS -

In this work, the dreiding forcefield was used for calculating the interactions between the different types of atoms and molecules.

HAMILTONIAN OF GENRIC FORCE FIELD

V = VΘ + VΦ + Vb + Vvdw + Velec

VΘ + VΦ + Vb = bonded.

V vdw + V elec = non bonded.

BOND STRETCHING ENERGY

$V = K (r1 - r2)^2 /2$

BOND BENDING ENERGY

$V = K(\theta 1 - \theta 2)^2$

BOND TORSION ENERGY

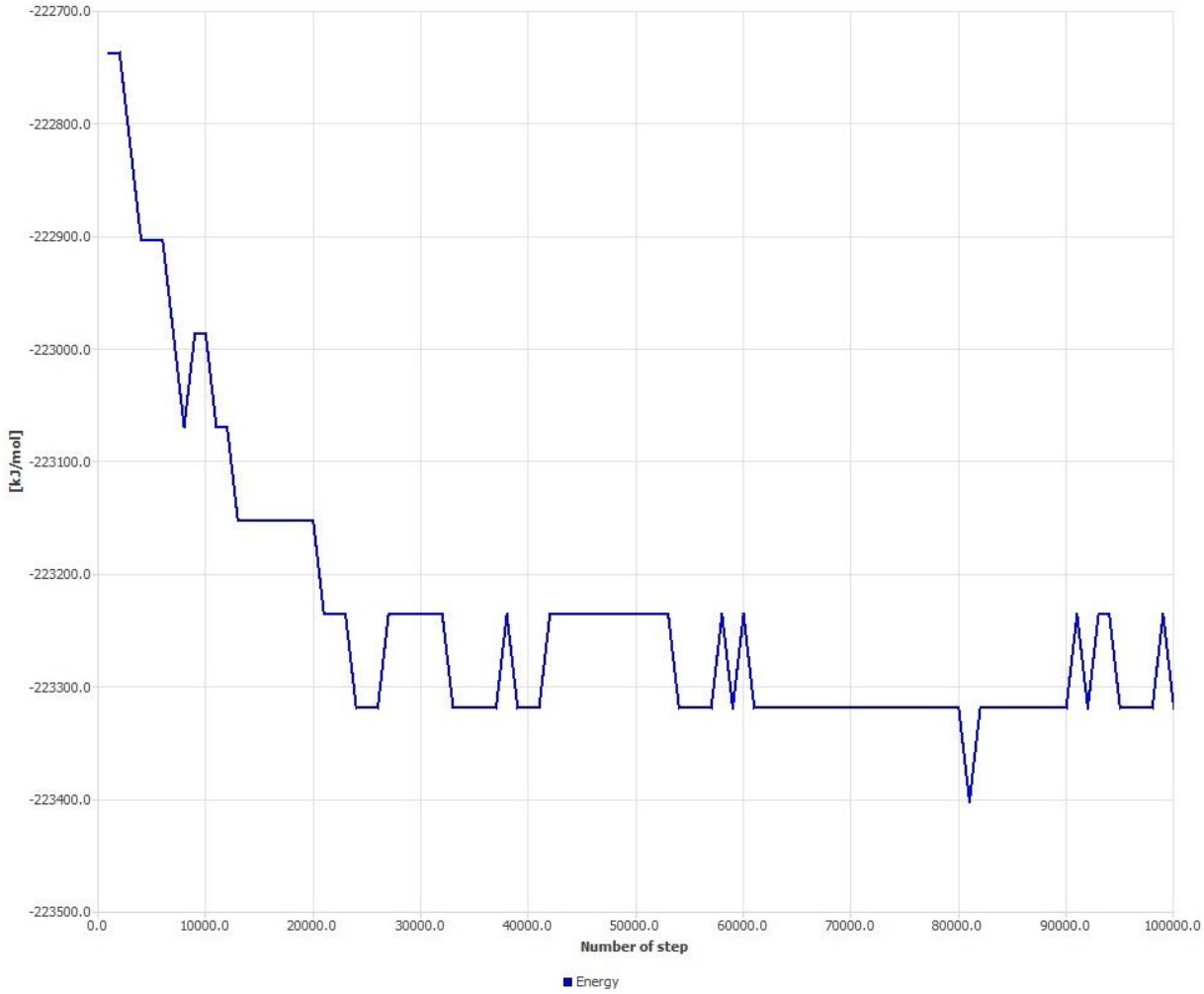
$V = K(1+ COS3\varphi) /2$

VAN DER WAALS ENERGY

V v dw(Rij)=4 { (R v dw / Rij)^12 - (R v dw / Rij) ^6 }

COULOMB'S LAW

*V elec = Q1.Q2/4π**ε**R*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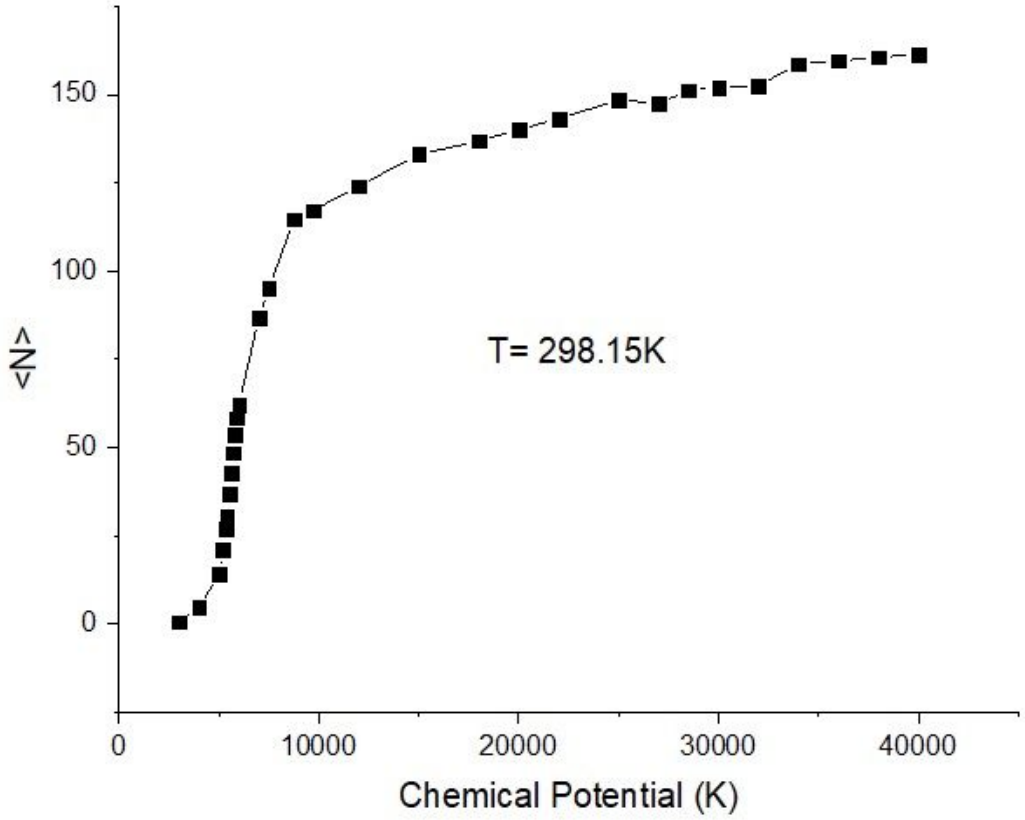
Energy



Adsorption Isotherm of Methane adsorped on Na-Faujasite