Simulasi Dinamika Molekuler Antarmuka (110) Gamma-Al2O3/H2O Menggunakan Metode Self-Consistent
Charge Density Functional Tight-Binding
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SIMULASI DINAMIKA MOLEKULER ANTARMUKA (110) γ-Al_2O_3/H_2O MENGGUNAKAN METODE *SELF-CONSISTENT CHARGE DENSITY FUNCTIONAL TIGHT-BINDING*

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INTISARI

Simulasi antarmuka (110) γ-Al_2O_3/H_2O dengan pendekatan *Self-Consistent Charge Density Functional Tight-Binding* (DFTB) dilakukan. Penelitian ini bertujuan untuk mempelajari proses adsorpsi dan disosiasi air pada permukaan (110) γ-Al_2O_3 dan sifat dinamik air pada antarmuka (110) γ-Al_2O_3/H_2O. Penelitian ini diawali ekuilibrasi (110) γ-Al_2O_3/H_2O dan dilanjutkan simulasi dengan *ensemble* NVT pada temperatur 298,15 K selama 20 ps. Analisis fungsi distribusi radial, disosiasi air, dan vibrasi molekul dilakukan untuk memperoleh gambaran dinamika air dalam antarmuka (110) γ-Al_2O_3/H_2O.

Informasi terkait dinamika adsorpsi dan disosiasi air berhasil diperoleh dari data simulasi yang dilaksanakan. Adsorpsi air pada permukaan (110) γ-Al_2O_3 dipicu atom aluminium pada permukaan tersebut, disertai proses disosiasi air, dan dilanjutkan dengan pembentukan ikatan antara oksigen pada permukaan (110) γ-Al_2O_3 dengan hidrogen dari molekul air terdisosiasi. Proses adsorpsi dan disosiasi menyebabkan perubahan distribusi dan karakter vibrasi air dalam antarmuka (110) γ-Al_2O_3/H_2O. Perubahan distribusi air digambarkan dengan puncak-puncak pada fungsi distribusi radial H dan O. Pembentukan ikatan hidrogen antara molekul air dengan oksigen permukaan ditandai puncak pada jarak 1,6 Å pada fungsi distribusi radial H. Puncak dengan jarak 2,0 Å pada fungsi distribusi radial O mengindikasikan terjadinya adsorpsi molekul air pada permukaan (110) γ-Al_2O_3. Terjadi pergeseran frekuensi vibrasi ulur OH akibat adsorpsi dan disosiasi air.

Kata kunci: antarmuka, dinamika molekuler, DFTB, gamma-alumina.

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MOLECULAR DYNAMICS SIMULATION OF (110) γ-Al_2O_3/H_2O INTERFACE USING SELF-CONSISTENT CHARGE DENSITY FUNCTIONAL TIGHT-BINDING METHOD

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ABSTRACT

Simulation of (110) γ-Al_2O_3/H_2O interface with Self-Consistent Charge Density Functional Tight-Binding approach was conducted. This research aims to study the process of water adsorption and dissociation on (110) γ-Al_2O_3 surface as well as the dynamics of water within the (110) γ-Al_2O_3/H_2O interface. The system was equilibrated and simulated in the NVT ensemble at 298.15 K for 20 ps. The radial distribution function, water dissociation, and molecular vibration were analyzed to study water dynamics within the (110) γ-Al_2O_3/H_2O interface.

Information regarding water adsorption and dissociation dynamics were obtained from simulation data. Water adsorption on (110) γ-Al_2O_3 surface is induced by surface aluminum atoms, followed by water dissociation, and results in the formation of bonds between surface oxygen and hydrogen atoms from dissociated water molecules. Adsorption and dissociation processes changed the distribution and vibrational properties of water within the (110) γ-Al_2O_3/H_2O interface. The change in water distribution is described by several peaks within the H and O radial distribution function. Hydrogen bond formation between water molecule and surface oxygen is denoted by a peak positioned at 1.6 Å in the radial distribution function of H. A peak positioned at 2.0 Å in the radial distribution function of O indicates the adsorption of water molecules on (110) γ-Al_2O_3 surface. The frequency of OH stretching shifts due to water adsorption and dissociation.

Keywords: DFTB, gamma-alumina, interface, molecular dynamics.