SIMULASI DINAMIKA DAN STRUKTUR TETRAGONAL ZIRKONIA (101) TERSULFATASI [SO_4^{2-}/ZrO_2] DENGAN METODE *SELF-CONSISTENT CHARGE DENSITY FUNCTIONAL TIGHT-BINDING* (SCC-DFTB)

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INTISARI

Penelitian struktur permukaan tetragonal zirkonia (101) tersulfatasi telah dilakukan. Penelitian ini dilakukan melalui simulasi dinamika molekular dengan metode *self-consistent charge density functional tight-binding*. Tujuan dari penelitian yaitu mempelajari struktur dan interaksi yang terjadi pada permukaan t-ZrO_2 (101) tersulfatasi (SO_4^{2-}/ZrO_2) serta mengidentifikasi vibrasi molekul pada permukaan t-ZrO_2 (101) tersulfatasi (SO_4^{2-}/ZrO_2).

Penelitian diawali dengan pemodelan struktur t-ZrO_2 dan t-ZrO_2 (101). Struktur t-ZrO_2 (101) hasil optimasi geometri diinteraksikan dengan H_2SO_4 dalam molekul H_2O. Simulasi dinamika molekular dilakukan selama waktu 20 ps. Metode SCC-DFTB yang digunakan dengan algoritma *Velocity Verlet* dan pengendali suhu termostat Berendsen.

Permukaan t-ZrO_2 (101) reaktif terhadap air dan sulfat. Interaksi permukaan t-ZrO_2 (101) dengan air membentuk ikatan Zr-OH_2, Zr-OH^-, dan >OH^+. Permukaan t-ZrO_2 (101) terjadi adsorpsi molekul SO_4^{2-} dengan ikatan monodentat, bidentat, dan tridentat. Vibrasi simetris molekul S-O pada bilangan gelombang 1002-1033 cm^{-1}, vibrasi asimetri S-O pada bilangan gelombang 1056-1095 cm^{-1}, vibrasi simetris S=O pada bilangan gelombang 1157-1165 cm^{-1} dan vibrasi asimetris S=O pada bilangan gelombang 1242-1257 cm^{-1}. Pada interaksi air, vibrasi *bending* H_2O pada bilangan gelombang 1513 cm^{-1} dan vibrasi regangan gugus OH pada bilangan gelombang 2950-3396 cm^{-1}.

Kata kunci: dinamika molekular, SCC-DFTB, zirkonia tersulfatasi.

SIMULATIONS OF DYNAMICS AND STRUCTURE OF SULFATED TETRAGONAL ZIRCONIA (101) [SO_4^{2-}/ZrO_2] BY SELF-CONSISTENT CHARGE DENSITY FUNCTIONAL TIGHT-BINDING (SCC-DFTB)

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ABSTRACT

Research into the surface structure of sulfated tetragonal zirconia (101) has been carried out. This research was conducted through molecular dynamics simulation using the self-consistent charge density functional tight-binding method. The purpose of this research was to study the structure and interactions that occur on the surface of sulfated t-ZrO_2 (101) (SO_4^{2-}/ZrO_2) and identify the molecular vibrations on the surface of sulfated t-ZrO_2 (101) (SO_4^{2-}/ZrO_2).

The study was initiated by modeling the structure of t-ZrO_2 and t-ZrO_2 (101). The structure of t-ZrO_2 (101) as a result of geometry optimization interacted with H_2SO_4 in the H_2O molecule. Molecular dynamics simulations were carried out for 20 ps. The SCC-DFTB method was used with the Velocity Verlet algorithm and the Berendsen thermostat as a temperature controller.

The surface of t-ZrO_2 (101) was reactive to water and sulfate. The surface interaction of t-ZrO_2 (101) with water forms Zr-OH_2, Zr-OH^-, and >OH^+ bonds. On the surface of t-ZrO_2 (101), adsorption of SO_4^{2-} molecules with monodentate, bidentate, and tridentate bonds occurred. S-O symmetrical molecule vibration at 1002-1033 cm^{-1}, S-O asymmetric vibration at 1056-1095 cm^{-1}, S=O symmetrical vibration at 1157-1165 cm^{-1} and S=O asymmetric vibration at 1242-1257 cm^{-1}. In the water interaction, the bending vibration of H_2O was at a wave number of 1513 cm^{-1} and the stretching vibration of the OH group was at a wave number of 2950-3396 cm^{-1}.

Keywords: molecular dynamics, SCC-DFTB, sulfated zirconia.