

**UNDERGRADUATE THESIS**

**ADSORPTION AND DISSOCIATION OF WATER AT THE  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> (110)  
SURFACE BY 2-DIMENSIONAL DENSITY-FUNCTIONAL BASED  
TIGHT-BINDING/MOLECULAR MECHANICS MOLECULAR  
DYNAMICS (2D-DFTB/MM MD) SIMULATION**

***ADSORPSI DAN DISOSIASI AIR PADA PERMUKAAN  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> (110)  
DENGAN SIMULASI 2-DIMENSI DENSITY-FUNCTIONAL BASED  
TIGHT-BINDING/MOLECULAR MECHANICS MOLECULAR DYNAMICS  
(2D-DFTB/MM MD)***



AHYA AULIA OKTARINI  
17/411471/PA/17865

**INTERNATIONAL UNDERGRADUATE PROGRAM OF CHEMISTRY  
DEPARTMENT OF CHEMISTRY  
FACULTY OF MATHEMATICS AND NATURAL SCIENCES  
UNIVERSITAS GADJAH MADA  
YOGYAKARTA**

**2021**