EFFECT OF TEMPERATURE CHANGE ON HYDROGEN ADSORPTION OF *α*-SiO2

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The ecological friendliness and sustainability of hydrogen energy have recently made it one of the most promising “green” fuels [1]. In particular, among these structures, SiO₂ based porous materials are potential candidates for hydrogen storage due to their harmlessness, low cost, and excellent thermal stability. Therefore, in this study, the effect of pore structures on the adsorption process of hydrogen molecules on *a*-SiO2 was investigated using molecular dynamics (MD) methods (Fig. 1. *a*). It can be seen from the results that the cooling rate plays a crucial role in changing the pore structure of *α*-SiO2, which in turn affects the sorption of hydrogen atoms and molecules (Fig. 1. *b*). The study showed that the maximum gravimetric density of hydrogen at 10 MPa is achieved at a cooling rate of 500 K/ps, where it reaches 0.92 wt% (8.45%).



Fig. 1. *a*) Hydrogens adsorbed on *a*-SiO2, *b*) Dependence of hydrogen gravimetric density on cooling rate at different pressures.

REFERENCES

1. R. Krishna et all., *Hydrogen storage for energy application*, in *hydrogen storage*, edited by j. Liu (intech, 2012).