

Abstract Submitted  
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**Energetics and Molecular Dynamics Simulations of Hydrogen Adsorption on a Silicon Nanosheet**<sup>1</sup> TIM H. OSBORN, AMIR A. FARAJIAN, Department of Mechanical and Materials Engineering, Wright State University, LOK C. LEW YAN VOON, Department of Physics, Wright State University, RACHEL AGA, Department of Chemistry, Wright State University — The energies and temperature-dependent dynamics of hydrogen chemisorption on a silicon nanosheet were studied using density functional theory and molecular-dynamics (MD) simulations. Energy calculations were performed by utilizing generalized-gradient approximation with the Perdew-Burke-Ernzerhof exchange correlation functional. The adsorption energies of hydrogen on the silicon nanosheet were calculated for different hydrogenation ratios corresponding to weight percents between 0 and 3.59 %. The preferred adsorption configurations were determined based on these energy calculations. MD simulations revealed the stability of adsorption configurations, and possible transitions between them, at different temperatures.

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