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Simulation of Hydrogen Diffusion in Hydrogenated Amorphous Silicon (a-Si:H) from ab-initio Molecular Dynamics F. GASPARI, A. SHKREBTII, J. PERZ, T. TEATRO, University of Ontario Institute of Technology, Oshawa, Canada, N. KHERANI, University of Toronto, Toronto, Canada — The role of hydrogen in hydrogenated amorphous silicon (a-Si:H) has been the subject of considerable studies in the past 30 years. In particular the mechanism of hydrogen diffusion and its relation to the bonding structure within the amorphous silicon network is considered to be crucial for the understanding of several properties of a-Si:H, including the Staebler-Wronski effect. We have investigated hydrogen diffusion in a-Si:H using first-principles molecular dynamics, by simulating a system of 64 silicon plus 10 neutral hydrogen atoms. The amorphous structure has been verified from the Radial Distribution Function. The dependence of the diffusion of the hydrogen atoms on different bonding configurations has been examined at different temperatures and the results have been correlated with experimental studies of hydrogen, deuterium and tritium effusion.

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