Simulations of Hydrogenated Amorphous SIlicon

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Hydrogenated amorphous silicon is an important material for myriad applications. Despite thirty years of intense experimental and theoretical research, important puzzles remain. For applications, the role of H in the network and photoresponse are of special importance. We describe the energetics and dynamics of both atomic and molecular hydrogen in realistic structural models. We then discuss thermally driven H hopping, and will emphasize the importance of the Si dynamics in determining hopping events. Photo-induced degradation of the material is modeled with a simple scheme to handle photo-excited network dynamics. By combining the results of these simulations with proton NMR measurements from Craig Taylor's group, it appears that the light-soaking leads to formation of particular dihydride configurations. These calculations are undertaken using the local orbital density functional code SIESTA.