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The Effects of Hydrogen on the Potential-Energy Surface of Amorphous Silicon JEAN-FRANCOIS JOLY, NORMAND MOUSSEAU, Universite de Montreal — Hydrogenated amorphous silicon (a-Si:H) is an important semiconducting material used in many applications from solar cells to transistors. In 2010, Houssem et al. [1], using the open-ended saddle-point search method, ART nouveau, studied the characteristics of the potential energy landscape of a-Si as a function of relaxation. Here, we extend this study and follow the impact of hydrogen doping on the same a-Si models as a function of doping level. Hydrogen atoms are first attached to dangling bonds, then are positioned to relieve strained bonds of fivefold coordinated silicon atoms. Once these sites are saturated, further doping is achieved with a Monte-Carlo bond switching method that preserves coordination and reduces stress [2]. Bonded interactions are described with a modified Stillinger-Weber potential and non-bonded Si-H and H-H interactions with an adapted Slater-Buckingham potential. Large series of ART nouveau searches are initiated on each model, resulting in an extended catalogue of events that characterize the evolution of potential energy surface as a function of H-doping.

[1] Houssem et al., Phys Rev. Lett., 105, 045503 (2010)
[2] Mousseau et al., Phys Rev. B, 41, 3702 (1990)

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