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Hydrogen microstructure of amorphous silicon via inversion of nuclear magnetic resonance spectra: A moment-based approach
PARTHAPRATIM BISWAS, The University of Southern Mississippi, RAJENDRA TIMILSINA, The University of Tennessee at Knoxville — We present an inverse approach for reconstructing hydrogen microstructure in amorphous silicon (a-Si). The approach consists of generating a prior distribution (of spins) by inverting experimental nuclear magnetic resonance (NMR) data, which is subsequently superimposed on a network of a-Si. The resulting network is then relaxed using a total-energy functional to obtain a stable, low-energy configuration such that the initial spin distribution is minimally disturbed. The efficacy of this approach is demonstrated by generating model configurations that not only have the correct NMR spectra but also satisfy simultaneously the experimental structural, electronic and vibrational properties of hydrogenated amorphous silicon.

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