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Self-trapping-enhanced carrier recombination at light-induced boron-oxygen complexes in silicon SHENGBAI ZHANG, MAO-HUA DU, HOWARD BRANZ, RICHARD CRANDALL, National Renewable Energy Laboratory — First-principles study of the BO_2 complex in B-doped Czochralski silicon reveals a self-trapping-enhanced carrier recombination mechanism that contrasts with the standard fixed-level Shockley-Read-Hall model for recombination. An O_2 dimer distant from the boron causes only a slow carrier recombination, which is, nevertheless, enough to drive the O_2 diffusion under light to form the BO_2 complex. We find that the BO_2 and O_2 produce nearly identical defect levels in the bandgap. Despite that, recombination at the BO_2 is substantially faster than that at the O_2, because the charge state of the latter inhibits a key step in the recombination, namely, the capture of the hole. This work was supported by the U. S. Department of Energy, BES and EERE, under Contract No. DE-AC39-98-GO10337.

Shengbai Zhang
National Renewable Energy Laboratory

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