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Stability and Dynamics of Frenkel Pairs in Silicon[1]

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Extensive EPR experiments on electron irradiated p-Si observe only signals identified as arising from isolated vacancies and interstitial impurities. Subsequent experiments and calculations demonstrated that isolated interstitials in p-Si diffuse athermally according to a charge-carrier- mediated mechanism. The overall conclusion has been that Si FPs either rapidly recombine or dissociate, even at cryogenic temperatures. More recent X-ray scattering experiments, however, suggest that Si FPs persist at temperatures up to 150 K. We report first-principles calculations of Si FP properties and resolve the apparent conflict between experiments. We find that the vacancy and interstitial components of a proximal FP interact electronically, suppressing the previously identified athermal interstitial diffusion. Such proximal FPs are bound only by the presence of barriers to either recombination or dissociation. Further, metastable FPs may lower their energy by transferring electrons from the interstitial to the vacancy component. We show that EPR studies of FPs are likely unable to distinguish between FPs and isolated vacancies. In addition, calculated diffusion barriers for FP components indicate that FPs should anneal at temperatures similar to those for isolated vacancies: $\sim$150 K.

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