Johnson, Herring, and Van de Walle Reply: Seager, Anderson, and Estreicher (SAE) [1] raise two kinds of questions about the validity of the conclusions of our Letter [2]: (1) Do our raw data describe correctly the response of Schottky diodes on hydrogenated n-type silicon to the various stimuli of pulsed hole injection and applied bias; and (2) does the H^0 formed in the process $H^- \rightarrow H^0 + e^-$ persist long enough as H^0 to achieve a distribution of lattice configurational coordinates close to that of H^0 in equilibrium? What SAE cite as our "assumptions" (a), (b), and the first part of (c) are *instead* direct statements of facts consistently observed in all our work [2–4]. A hole pulse followed by a sweepout transition has in our work always produced a permanent rise in the active-donor profile, proportional to the hole dose at low doses; the reversibility described by SAE has not been observed with our diodes and measurement conditions. The fact that the initial capacitance change is very close to twice that after sweepout indicates that a mobile charge (H^+) and a fixed charge (P^+) are produced at nearly the same place and that the former is swept out without retrapping. The fact that a prompt electron flooding pulse, which cannot affect the new P^+, always reduces the initial capacitance change almost to zero directly demonstrates the conversion of the new H^+ to H^-. Incidentally, our production of isolated, monatomic hydrogen was confirmed by our observation of the generally-accepted deep-level transient spectroscopy signature for the donor level ($E3'$) [4].

SAE assert that in many experiments on hydrogenated n-type silicon diodes they have never observed hole-induced transients of the types reported by us. This contrasts markedly with our experience: We have measured scores of capacitance transients on numerous diodes and under a wide range of measurement conditions (e.g., temperature, bias, and PH density), every one of which has shown the same key features as those in [2–4]. (The P density has usually been near 10^{16} cm^{-3}, because remote-plasma passivation is less effective at lower doping while at much higher dopings sweepout becomes so fast as to obscure the effects of the $H^- \rightarrow H^+$ charge change.)

One possibility for the differences observed by SAE is their suggestion that their samples may contain traps that can capture monatomic H and become positively charged, eventually releasing it to passivate a nearby P^+. We think it unlikely that they observed appreciable formation of PH^+, with subsequent slow conversion to PH by electron capture, since if so this mechanism should have produced at least a measurable effect in our work.

We *explicitly* assumed that when H^- spontaneously converts to H^0 it usually moves as H^0 to the vicinity of the BC site before converting to H^+ [2]. There are experimental and theoretical indications that this assumption is probably correct. If H^0 could be metastably trapped near the T_d site at low temperatures it would produce a characteristic electron spin resonance, which

while sought [5] has never been found. From theory, our assumption should be valid if the adiabatic energy surface for H^0 has a form close to that shown in our Fig. 3, which was obtained from electronic total-energy calculations based on the density-functional technique. We have confirmed these results by using a more refined code which allows a thorough exploration of the energy surface with a larger basis set: The BC site is the most stable, and the energy surface around T_d does not exhibit any additional local minima (to within an accuracy of 0.1 eV). SAE argue that other computational schemes give different results. However, the failure of the cited quantum-chemistry-based methods to identify H^- as a stable species [6] casts doubt on the ability of such methods to describe the energy surface near T_d. The density-functional calculation has been very successful on a wide variety of problems when carried out with a sufficiently large basis.

The impressive results from studies of muonium in silicon are in no way inconsistent with the adiabatic potential energy curves shown in our Fig. 3. A recent calculation [7] of the possible states of muonium moving as a quantum-mechanical particle in a dynamic silicon lattice shows how an adiabatic potential similar to ours can yield a ground state in which the muonium spends most of its time near the T_d site, even though the adiabatic potential at T_d (after local relaxation) is much higher than at BC. This is because the potential is much flatter in most directions near the T_d site. Interestingly, too, the calculation also found a metastable site for muonium at low temperatures, presumably because it is difficult for a light particle to squeeze through a narrow path. Thus, there is no fundamental inconsistency with a potential which allows a heavy particle (deuterium) to coast downhill from T_d to BC and a light particle (muonium) to be localized near T_d.

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