Open Question to Point Defects

Von G.F. Cerofolini (1989):

Having recently written a book on physical chemistry of, in and on silicon [1], I have considered some of the most obvious queries which could be raised when considering such a topic, viz.:

1. which is the atomic configuration of point defects? (e.g., is the self- interstitial quasi free or does it have a dumb-bell configuration?)
2. has each defect only one configuration or are several configurations possible?
3. which is the electronic structure?
4. which charge states are associated with each defect and where are they located in the gap?
5. can the defect be actually considered pointlike (i.e., do the remaining atoms remain on their lattice location) or does the deformation extend to long range?
6. does an entropic or enthalpic barrier exist for Frenkel-pair recombination?
7. which are the defect diffusivities in relation to their charge states?
8. is the surface an effective generation-recombination centre for point defects?
9. to which extent does this generation-recombination rate depend on surface conditions (free, oxidated, nitridated, etc.)?

Most of them, however, remained unanswered.

Advanced