Supplementary Information: Ultrafast Palladium Diffusion in Germanium

Figure S1(a) and (b) show the DOS for the split- V_{Ge} configuration. {Pd-split- V_{Ge} }⁻¹ shows states due to Ge above the Fermi level. This modifies the top of the valence band by introducing Ge *p*-states and Pd *d*-states into the band gap causing it to shrink to 0.38 eV. For high Pd concentrations (~1.6 %) as encountered in this study, such modification of the band gap would be detrimental to semiconductor device operation, in the dilute limit, however, the impact of a single Pd atom will normally be negligible. After the transition to charge -2 the Ge electronic structure is retained and the band gap recovers with the absence of any states within the band gap. This is also the case for Pd_i which shows no states within the band gap and maintains the calculated band gap of 0.65 eV.





(e) Pd_{Ge}^{-1}

Figure S1 | **Partial densities of states.** The partial densities of states for the Pd defects in Figure 1 of the main article in increasing order of stability.