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Isotope effect in the vibrational lifetime of the CH_2^* defect in Si MICHAEL GIBBONS, STEFAN ESTREICHER, Texas Tech University, MICHAEL STAVOLA, Lehigh University — The CH_2^* defect in Si has two metastable configurations with H bound at bond-centered (BC) or antibonding (AB) sites of Si and C: Si-H_{BC}...C-H_{AB} or H_{AB}-Si...H_{BC}-C. Th IR absorption signature of this defect should consist of four sharp lines associated with the two Si-H and two C-H stretch modes, respectively. Yet, only three modes have seen by FTIR, and the fourth, very broad, line has only recently been reported by the highly sensitive multiple-internal-reflection FTIR. Further, the "missing" mode produces a very sharp line only for the deuterium substitution Si-H_{BC}...C-D_{AB}. Our calculations show that this is due to the isotope-dependence of the vibrational lifetime of this mode. The C-H mode decays very quickly into two phonons and the very short lifetime causes the IR line to be extremely broad. On the other hand, the C-D mode has a much longer lifetime and decays into at least three phonons, resulting in a much sharper IR line. We will report the calculations of these vibrational lifetimes.

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