

OPTICALLY ACTIVE HYDROGEN DIMERS IN SILICON

B. Hourahine,¹ R. Jones,¹ A. N. Safonov,² S. Öberg,³ and P. R. Briddon⁴

¹School of Physics, The University of Exeter, Stocker Road, Exeter, EX4 4QL, U.K.

²Department of Physics, University of Durham, South Road, Durham, DH1 3LE, U.K.

³Department of Mathematics, University of Luleå, Luleå S-97187, Sweden

⁴Department of Physics, The University of Newcastle upon Tyne, Newcastle upon Tyne, NE1 7RU, U.K.

Key Words: Hydrogen, Dimers, Silicon, Photoluminescence

Under certain conditions in crystalline silicon hydrogen is known to form photoluminescence centres with some unusual characteristics. In particular, B_{41} and B_{71}^1 centres, which appear in hydrogenated silicon after irradiation and subsequent thermal treatment, were shown to contain two hydrogen atoms with trigonal symmetry and to produce shallow localised states near the conduction band edge [1].

It is not easy to construct a credible model for such defects. We report the results of first principles calculations on V_6H_2 , which has properties consistent with those of B_{41} . The H atoms are not bonded together, but are attached to the Si lattice. The results of the calculations suggest that B_{41} and B_{71}^1 is formed due to conversion of V_6 into V_6H_2 defects during thermal treatment. We consider also results supporting the link between V_6 and B_{71}^1 defects. Tentative assignments to other similar PL centres are given.

[1] A. N. Safonov, E. C. Lightowers and G. Davies, Phys. Rev. B **56** 15517 (1997).