WHY DO DIVACANCIES DISTORT IN SEMICONDUCTORS?

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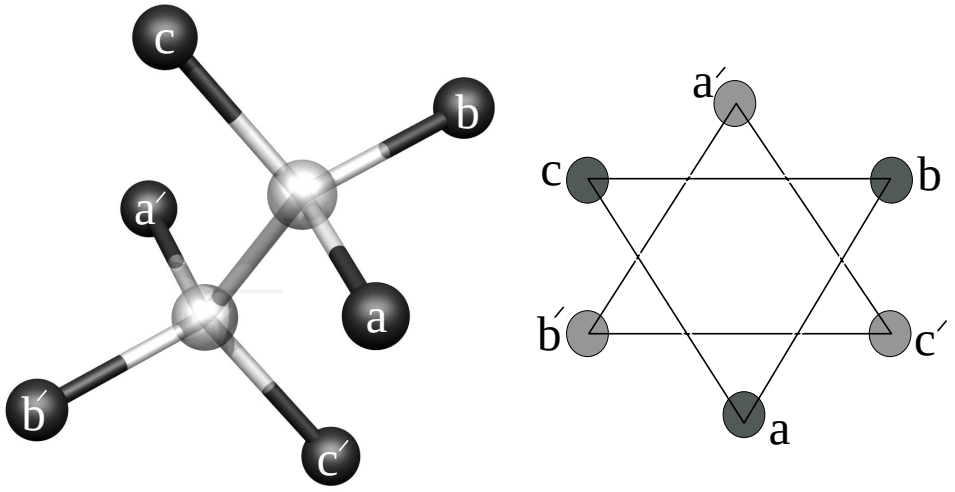
Recent density functional calculations reveal a distortion of the divacancy in silicon at variance with experimental results. The subtle nature of the bonding processes involved has evidently proved a demanding task for computational modelling. The observation of a distorted structure (C_{2h}) for the divacancy in diamond despite its non-degenerate electronic ground state is equally puzzling since a Jahn-Teller distortion requires ground state degeneracy. We report on large scale, *ab initio* calculations on these divacancies in both silicon and diamond which result in distortions consistent with experiment and highlight inadequacies of earlier modelling studies.

Spin-polarised local density functional cluster theory is employed in this study. In both silicon and diamond we can summarise the possible models in three distinct structures. The ideal structure (see figure) possesses D_{3d} symmetry. Two distortions are also investigated, both resulting in a structure with C_{2h} symmetry. The first involves a *pairing* of bonds across the divacancy (so that atom pairs b and c, and b' and c' form bonds). The second is a distortion of the opposite sign (*i.e.* atom pairs b and c, and b' and c' move apart). The distinct electrical, optical and magnetic properties of each model allows clear identification with observed centres.



ABOVE: A schematic diagram of the divacancy.

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