AB INITIO INVESTIGATION OF OXYGEN DEFECTS IN Si

C. Ewels[a], R. Jones[a] and S. Öberg[b]

[a] Department of Physics, University of Exeter, Exeter, EX4 4QL, UK
[b] Department of Mathematics, University of Luleå, Luleå, S95187, SWEDEN

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Ab initio techniques are used to study vacancy oxygen complexes in Si. Substitutional oxygen is found to be an off-site defect in agreement with experiment. It possesses one high frequency O-related LVM at 788 cm^{-1} in good agreement with an assigned mode at 831 cm^{-1}. The VO_2 defect is found to possess D_{2d} symmetry and only one O-related high frequency IR active mode at 807 cm^{-1}. The VO_3 defect has three high frequency IR active modes lying above the LVM for VO_2. The calculated frequencies are in fair agreement with those tentatively assigned to VO_3 at 1005, 976 and 910 cm^{-1}. On the other hand, the V_2O defect has one such LVM at 790 cm^{-1}. These results provide support for the assignment of the 889 cm^{-1} (300 K) local vibrational mode to VO_2 rather than to V_2O.

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